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DEVELOPMENT OF A COMPUTER-BASED AIR FORCE INSTALLATION RESTORATION WORKSTATION FOR CONTAMINANT MODELING AND DECISION-MAKING

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The objective of this research is to develop a groundwater remediation advisory system for use in investigating possible remediation activities for the cleanup of contamination from hazardous substances, pollutants and contaminants at Air Force sites. The advisory system provides a decision framework for selecting an appropriate model from the numerous available transport models conditioned on available site data. In addition, the use of optimization methods is explored for determining optimal remediation strategies at a specific site. The optimization routine evaluates tradeoffs between the long-term cost of remediation and the probability the remediation strategy will fail. The final product of this project is a computer-based Air Force Installation Restoration Workstation Advisory System for contaminant modeling and decision-making. This software can be used as an aid to technical project managers within the U.S. Air Force Installation Restoration Program in developing and evaluating possible remediation alternatives and managing ongoing remediation activities.

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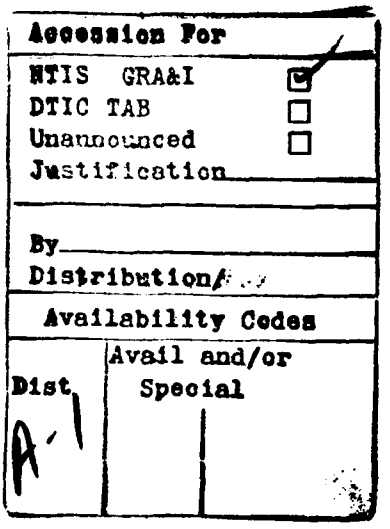
PREFACE

The research described in this report was conducted by Drs. Miguel A. Medina, Jr. and Timothy L. Jacobs, Department of Civil and Environmental Engineering, Box 90287, Duke University, Durham, North Carolina 27708-0287, under Contract F08635-92-C-0009, under the sponsorship of the Headquarters Air Force Engineering and Services Center, Engineering and Services Laboratory (HQ AFESC/RD), and Armstrong Laboratory Environics Directorate, Tyndall AFB, FL 32403-6001. The Project Officer was Dr. Tom Stauffer (HQ AFESC/RAVC).

This research was performed between November 15, 1991 and December 15, 1992.

Several meetings were held at Headquarters Air Force Center for Environmental Excellence (HQ AFCEE), Brooks AFB, Texas and Headquarters Air Force Engineering and Services Center (HQ AFESC), Tyndall AFB, Florida to solicit comment from potential users. The principal investigators wish to acknowledge the valuable suggestions received from representatives of Tinker AFB, Kelly AFB, Hill AFB, Brooks AFB, Tyndall AFB and MITRE Corporation.



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EXECUTIVE SUMMARY

The objective of this research is to develop a groundwater quality modeling advisory system for use in investigating possible remediation activities for the cleanup of contamination from hazardous substances, pollutants and contaminants at Air Force sites. In addition, this research explores the use of optimization methods for determining optimal remediation for implementation at a specific site. A 1987 Executive Order authorized the Secretary of Defense to implement the Department of Defense Installation Restoration Program (IRP). The objectives of this program include the identification, investigation, research and development, and cleanup of sites contaminated with hazardous substances from past and present activities. The Air Force has established its own in-house management and technical expertise for implementing, monitoring and managing activities within the IRP. The remedial action process consists of four discrete processes. These include: (1) Preliminary Assessment and Site Inspection, (2) Remedial Investigation and Feasibility Study, (3) Remedial Design and Remediation Action and (4) Site Closeout. The focus of the research summarized in this report impacts the implementation of the Remedial Investigation and Remedial Action phases of the remedial action process.

Over the past several decades, many different models for contaminant transport in porous media, under varying conditions and assumptions, have been proposed and tested. These range from very simple models based on one-dimensional analytical solutions, which assume a completely homogeneous and isotropic medium, to very complex models based on three-dimensional numerical solutions which allow for complete specification of the aquifer and contaminant characteristics throughout a three-dimensional grid. All contaminant transport models, regardless of the complexity of the solution method, require certain assumptions regarding the nature of the transport processes, and, therefore, can only approximate the actual spread of contaminants from a given site and the associated risks from human exposure to contaminated groundwater.

This situation presents a familiar, yet difficult problem to the analyst and the decision-makers. Sufficient data on the hydrogeology are rarely, if ever, available to apply the most complex, three-dimensional contaminant transport models to a proposed or monitored site. The analyst must choose a transport model based on a tradeoff between the presumed greater accuracy of complex models and the less onerous data requirements and easier application of simpler models. The topic of choosing an appropriate model is one of the important aspects of the advisory system under development for the Air Force, and specific algorithms have been developed to assist the user with this task.

Even with the choice of an appropriate transport model, considerable uncertainty is likely to be present in the analysis of contamination risk. Application

of groundwater transport models requires estimation of parameters which are both difficult to measure and spatially variable, such as hydraulic conductivity and dispersivity. There is often good reason to doubt the accuracy of the input data. For instance, if an analytical model requires the spatial average of the hydraulic conductivity throughout the local area of the aquifer, and the available data consist of only one or two slug tests, plus perhaps an expert opinion, there is good reason to doubt that the reported best estimate of the parameter accurately reflects the true mean value. Simply running the model in a deterministic mode using the best estimates of the parameters may not provide sufficient information for a decision, because the uncertainty in the analysis has not been taken into account. For instance, if a deterministic application suggests no risk of contamination, no information is provided as to the certainty of this conclusion.

The recommended alternative is to explicitly consider the uncertainty in the analysis, through the use of Monte Carlo analysis. Uncertainty enters the modeling process in three ways: (1) through natural parameter variability; (2) through measurement error, which also introduces uncertainty in parameter estimation; and (3) through model error, representing uncertainty introduced by the degree to which the simplifying assumptions used to develop a model fail to accurately represent the actual physical processes at the site in question. The first two of these sources of uncertainty can be analyzed separately. However, the data are often insufficient: in such cases, the natural and measurement uncertainty may be combined into one source of uncertainty for the Monte Carlo analysis, through the specification of the distribution of the parameter value.

The third source of uncertainty in the analysis is due to the degree to which the transport model applied may misrepresent actual processes at the site. Examples of this source of uncertainty include the sorption of contaminants to soil surfaces and degradation rate coefficients. This source of uncertainty is very difficult to quantify, and indeed may be impossible to quantify for specific sites, unless extensive sampling and monitoring data are available.

A Monte Carlo analysis requires that distributions be specified for the underlying parameters having the greatest impact on contaminant transport. Specification of a parameter distribution consists of two steps: (1) choice of a distributional form, and (2) specification of the descriptive parameters of that distribution. On the first issue, the choice of distributional form, the system does of necessity provide some limitations. That is, for models which are expected to be used in cases for which the impacted aquifer is at least moderately well-characterized, certain parameter distributions are constrained to follow specific forms, which are generally well accepted in the literature. For instance, in some of the models the mean hydraulic conductivity must be specified by a log-normal distribution. However, even in these cases, a choice is present in the parameterization, as the mean hydraulic conductivity may be directly specified from the log-normal, or generated from underlying parameter

distributions. In general, where the parameters are at least moderately well known the choice of a distributional form should not have a major impact on the results. In its present form, the Advisory System incorporates the framework for Monte Carlo analysis, but additional research is needed to develop the parameter distributions and values for site-specific hydrogeologic conditions.

In addition to aiding in the choosing of an appropriate mathematical model for a specific site, the Advisory System is being modified to determine efficient or optimal remediation strategies. The optimization routine evaluates tradeoffs between the long-term cost of remediation and the probability the remediation strategy will fail.

A chance-constrained optimization model is being developed to determine the most efficient groundwater remediation strategies. The optimization model is multiobjective and driven by probabilistic measures of contaminant concentration in the groundwater surrounding the hazardous waste site. The chance-constrained model is used to determine the tradeoffs that exist between short-term and long-term remediation costs and the probability that the remediation strategy will fail.

The development of an efficient, effective and reliable remediation strategy requires a clear understanding of the site characteristics and the remediation actions implemented. In addition, the optimal remediation strategy must consider tradeoffs between the remediation cost and the reliability of the remediation strategy. By investigating these tradeoffs, the decision maker can more accurately assess remediation needs, feasible remediation strategies and remediation strategy effectiveness.

Long-term remediation costs depend on specific remediation considerations and actions. Examples of possible remediation strategies include pulse pumping and treatment, and continuous pumping and treatment. Potential cost savings are realized by varying the long-term remediation action. The reliability of the long-term remediation strategy represents the likelihood that contaminant concentrations within the groundwater exceeds specified maximums and are modeled as constraints. These two conflicting goals or objectives are weighed against one another, using a chance-constrained optimization model in which the physical constraints are originally expressed as probabilistic statements.

Using this methodology, optimal groundwater remediation strategies are determined by minimizing the long-term and short-term costs associated with the site remediation. In addition, the optimal remediation strategies are conditioned on the probability that the contaminant concentration at any time does not exceed pre-specified maxima. The actual concentrations at any specified coordinates are calculated by solving the governing differential equations for groundwater contaminant flow in which key site characteristics are expressed as random variables. The resulting optimization model is solved using a second moment formulation combined

with Monte Carlo simulation.

The final product of this project is a computer-based Air Force Installation Restoration Advisory System Workstation for contaminant modeling and decision making. When completed, the Advisory System will be fully documented and compatible with the DOS and UNIX operating systems. This software can be used as an aid to technical project managers within the U.S. Air Force Installation Restoration Program in developing and evaluating possible remediation alternatives and managing ongoing remediation activities.

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INTRODUCTION

A. OBJECTIVES

Air Force needs for contaminant transport mathematical modeling and decision-making, in terms of the predictive requirements of the Installation Restoration Program (IRP), may at least be partially addressed by development of an interactive, user-friendly computer-based engineering workstation. Background information on Department of Defense environmental restoration efforts and, specifically, the Air Force IRP is presented in the next section. The principal element of the workstation is an advisory system incorporating basic software to: define the magnitude, extent, direction, and rate of movement of identified contaminants; identify significant public health and environmental hazards of migrating pollutants; recommend candidate remedial actions; maintain databases of model parameters, and accomplish other supporting tasks. The principal function of a workstation is to provide optimal and efficient support to its user regarding the tasks determined for the user/workstation entity. Generally, this function can be divided into a number of subfunctions which are determined by analyzing the tasks performed by the intended users and the hardware/software environments available. Important elements in this analysis are determining the amount and type of data and establishing the level of synthesis required to adequately perform the required tasks. Furthermore, the various levels of expertise of potential users must be determined and accommodated for in the operating system to provide users with adequate assistance.

B. BACKGROUND

The legal mandate for the Air Force (AF) Installation Restoration Program (IRP) is the Comprehensive Environmental Response, Compensation and Liability Act of 1980 (CERCLA, known as the Superfund Act) and the Superfund Amendments and Reauthorization Act of 1986 (SARA). Section 211 of SARA deals with the Defense Environmental Restoration Program (DERP), of which the IRP is the primary subcomponent (Reference 1). A 1987 Executive Order provided authority to the Secretary of Defense to implement the Department of Defense (DOD) Environmental Restoration Program within the overall framework of CERCLA and SARA. The objectives of the IRP include "the identification, investigation, research and development, and cleanup of contamination from hazardous substances, pollutants, and contaminants." The program is focused on cleanup of detected contamination from past activities, but as noted includes research as well as development and demonstration of innovative and cost-effective cleanup technologies. IRP activities are managed centrally in the Office of the Secretary of Defense and are carried out by the

Military Services and Defense Agencies. Under this agreement, the U.S. Air Force retains the authority and initiative for cleanup activities at its own installations.

The Air Force has established its own in-house management and technical expertise for implementing the IRP, following a decentralized approach which places emphasis and authority with the Major Air Commands (MAJCOMs) and, in turn, with the individual installations under their jurisdiction (Reference 2). Several service organizations support the implementation of the Air Force IRP: the Air Force Civil Engineering Support Agency (AFCESA, HQ at Tyndall AFB, Florida), Armstrong Laboratory Environics Directorate, Tyndall AFB, Florida, the Center for Environmental Excellence (AFCEE, Brooks AFB, San Antonio, Texas), and the AF Regional Civil Engineer offices. Additional support is provided by the Air Force Material Command (AFMC), which is responsible for the advancement and effective management of the Air Force scientific and technical resources. An Air Force Installation Restoration Management (AFIRM) Committee has also been organized to support the MAJCOMs and review remedial action plans for complex problems.

The remedial action process is a progression of steps designed to fully analyze and address site problems, grouped functionally by stages, as follows:

1. Preliminary Assessment/Site Inspection (PA/SI) Stage,
2. Remedial Investigation/Feasibility Study (RI/FS) Stage,
3. Remedial Design/Remedial Action (RD/RA) Stage,
4. Site Closeout (SC) Stage.

Figure 1 illustrates these four stages and 14 steps of the remedial action process. The opportunity for application of contaminant transport models arises primarily in the second (investigation) and third (cleanup) stages. However, mathematical models may be used in the first stage in the case of unknown subsurface sources of contamination: the most likely location of the source could be calculated from known field measurements of the edge of the plume — as part of the discovery and preliminary assessment steps.

In the second stage, mathematical models may be applied to:

- Estimate the rate and extent of contamination migration from several sources (surface and subsurface);
- Simulate current and future scenarios of contamination and potential impacts at all locations of interest;
- Evaluate the likely effectiveness of proposed alternatives for remediating the impacts of released contaminants;

- Perform risk analysis, accounting for uncertainty in predictions, to assist in selection of the best remedial strategy.

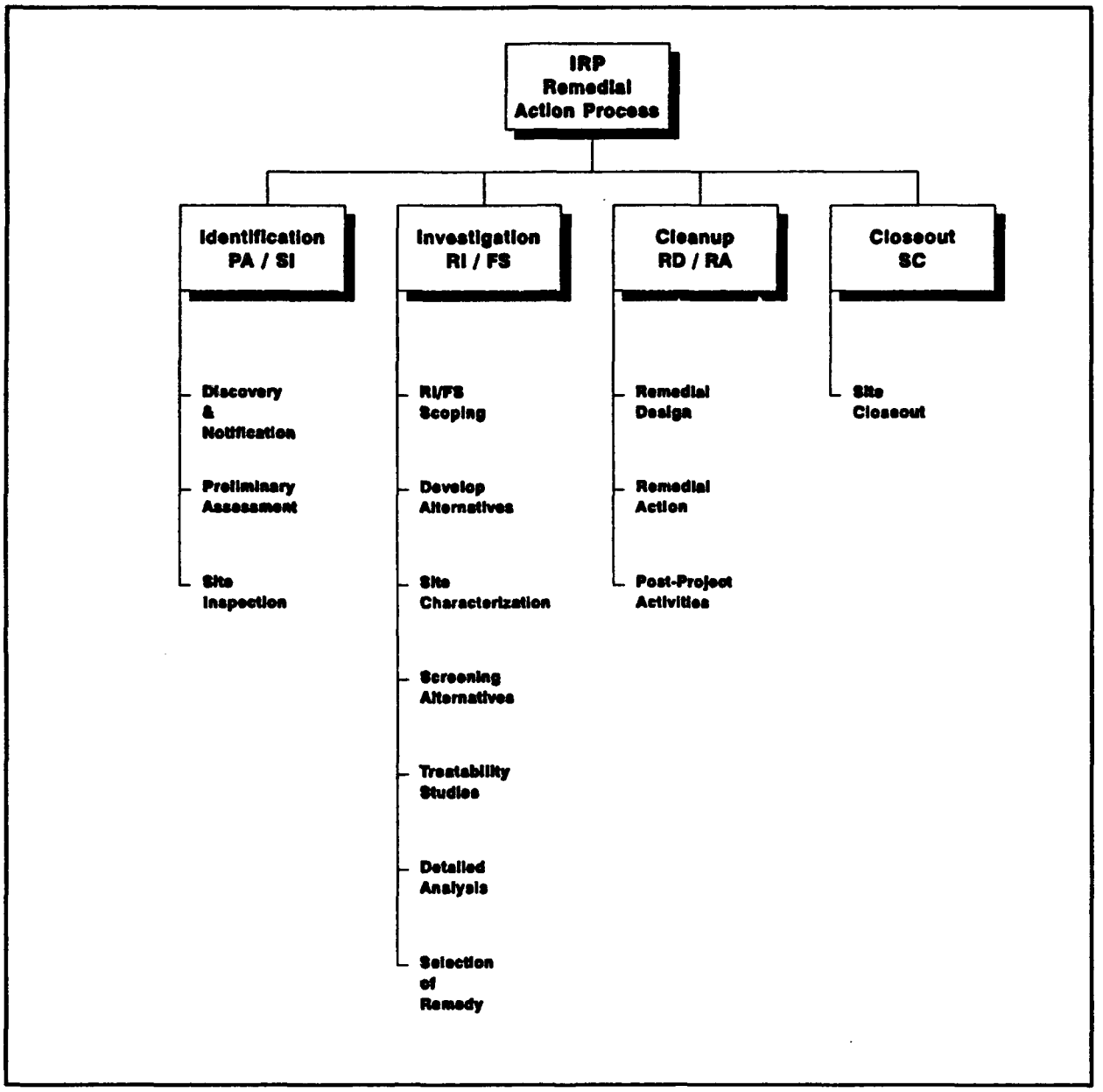


Figure 1. IRP Remedial Action Process

In the third stage (cleanup), models are useful in designing the remedial strategy: the optimal strategy should be cost-effective. Models do not reduce the

need for good quality site-specific data: they help determine data needs, make better use of available data, and refine the data collection (monitoring) process to insure compliance with cleanup goals.

The Air Force Center for Environmental Excellence (AFCEE) at Brooks AFB (San Antonio, Texas) operates the technical information management system (IRPIMS) for Air Force IRP sites. It is one of the contract support centers for investigative studies. It can provide technical consultation, field monitoring, sample analysis support, and has developed programs on site ranking and Quality Assurance/Quality Control (QA/QC).

C. SCOPE

Seven groundwater models and one surface water quality model are maintained within IRPIMS. However, these models need updating, do not have the capability of addressing uncertainty in model prediction, are not integrated within a decision-analysis framework, and do not address many of the complex flow and mass transport phenomena exhibited by solvents in groundwater.

Advisory systems provide a systematic framework for the determination of optimal choices independent of (but interacting with) the transport models employed for concentration calculations. The conceptual structure of such systems incorporates several premises:

1. The best decisions are made by technically informed individuals which may be aided by computer-based data handling and analysis,

2. Synthesis of technical, socio-economic and political aspects may be necessary;

3. Problem visualization through high-resolution graphics facilitates insight and problem comprehension;

4. Guidance and problem representation assistance, not dictated decisions, provide optimal decision support;

5. The central role of the human decision maker requires that decision support tools be designed as man-machine systems.

A workstation may include both surface and groundwater models, aimed at developing alternative remediation strategies for polluted surface and groundwater systems, and at designing the technical details of a preferred remedial action. It should be designed to perform:

1. Data management and analysis

    a. Acquisition of data directly from the field, from maps, and from other databases;
    b. Data reduction;
    c. Data analysis;
    d. Data storage and retrieval; and
    e. Graphical presentation of data.

2. Site characterization

3. Source identification

4. Plume delineation

5. Contaminant transport analysis

6. Risk analysis

7. Evaluation and optimization of potential remedial action alternatives, compliance monitoring, sampling strategies

Its components should include:

1. Hardware

    a. Graphics capability
    b. Peripherals (e.g., printer, mouse)
    c. Communication links
    d. Storage devices

2. Software

    a. Data storage, management, analysis
    b. Simulation models
    c. Hydrogeologic, hydrogeochemical analysis
    d. Shell: user-friendly interface
        i. help screens
        ii. advisory system interface
        iii. database of model parameters
        iv. linkage to IRPIMS, graphics

In designing the workstation, flexible architecture is necessary for efficient updating, maintenance, and expansion of hardware and software. In addition, an

operational support structure needs to be implemented for the system maintenance and to provide user-application support. Finally, as an integral part of the organizational workstation environment, a continuing technology transfer program should be developed to include general introduction courses, various levels of on-site hands-on training, and roving experts visiting the different workstation locations on a regular basis.

SECTION II

METHODOLOGY

A. ROLE OF UNCERTAINTY IN GROUNDWATER RISK ANALYSIS

Over the past several decades many different mathematical models for contaminant transport in porous media have been proposed and tested, under varying conditions and assumptions. These range from models based on closed-form analytical solutions to one-, two- and three-dimensional versions of the governing differential equations (assuming completely homogeneous and isotropic media), to highly complex numerical solutions of equations which allow for complete specification of both the aquifer and the contaminant characteristics throughout a three-dimensional grid. All of these contaminant transport models, regardless of the complexity of the solution method, require certain assumptions regarding the nature of the transport processes and the physical system abstracted, and so can provide only an approximation of the actual spread of the contaminant(s) from a given site and the associated risk.

This situation presents a familiar, yet difficult problem to the analyst and the decision-makers. Sufficient data on the hydrogeology are rarely available to apply the most complex, three-dimensional flow and contaminant mass transport models to even well monitored sites. The analyst must, whether explicitly or implicitly, choose a transport model based on a trade-off between the presumed greater accuracy of complex models and the less onerous data requirements and easier application of simpler models. The topic of choosing an appropriate model is one of the important aspects of the advisory system under development for the Air Force.

Even with the choice of an appropriate code-verified transport model, considerable uncertainty is likely to be present in the analysis of contamination risk. In groundwater transport models (which require estimation of parameters which are difficult to measure and spatially variable, such as hydraulic conductivity and dispersivity), there is often good reason to doubt the accuracy of the input data. For instance, if an analytical model requires the spatial average of the hydraulic conductivity throughout the local area of the aquifer, and the available data consist of only one or two slug tests, plus perhaps an expert opinion, there is good reason to doubt that the reported best estimate of the parameter accurately reflects the true mean value. Simply running the model in a deterministic mode using the best estimates of the parameters will not then provide sufficient information for a decision, because the uncertainty in the analysis has not been taken into account. For instance, if a deterministic application suggests no risk of contamination, no information is provided as to the certainty of this conclusion.

The recommended alternative is to explicitly consider the uncertainty that is present in the analysis, through the use of stochastic methods such as Monte Carlo analysis. Uncertainty enters the modeling process in three ways: (1) through natural parameter variability; (2) through measurement error, which also introduces uncertainty in parameter estimation; and (3) through model error, representing uncertainty introduced by the degree to which the simplifying assumptions used to develop a model fail to accurately represent the actual physical processes at the site in question. The first two of these sources of uncertainty can be analyzed separately. However, the data are often insufficient: in such cases the natural and measurement uncertainty may be combined into one source of uncertainty for the Monte Carlo analysis, through the specification of the distribution of the parameter value.

The third source of uncertainty in the analysis is due to the degree to which the transport model applied may misrepresent actual processes at the site. This source of uncertainty is unfortunately very difficult to quantify, and may indeed be impossible to do so for specific sites unless extensive sampling and monitoring data are available.

To conduct a Monte Carlo analysis, it is required that distributions be specified for the underlying parameters. Specification of a parameter distribution consists of two steps: choice of a distributional form, and specification of the hyperparameters of that distribution. On the first issue, the choice of distributional form, the system does of necessity provide some limitations. That is, for models which are expected to be used in cases for which the impacted aquifer is at least moderately well characterized, certain of the parameter distributions are constrained to follow specific forms, which are generally well accepted in the literature. For instance, in some of the models the mean hydraulic conductivity must be specified by a log-normal distribution. However, even in these cases a choice is present in the parameterization, as the mean hydraulic conductivity may be directly specified from the log-normal, or generated from underlying parameter distributions. In general, where the parameters are at least moderately well known the choice of a distributional form should not have a major impact on the results. In its present form, the workstation Advisory System incorporates the framework for Monte Carlo analysis for several models, but additional research is needed to develop the required parameter distributions and values for site-specific hydrogeologic conditions.

Once a specific transport model is selected, an estimate of the unconditional distribution of the contaminant concentration is needed to assess the risk associated with a site. The resulting unconditional contaminant concentration distribution is then utilized to assess the risk associated with a specific site using Bayes' theorem. For example, if variabilities are considered in the time to the waste container failure, the actual leachate release concentration and the spatial variation of the hydraulic conductivity, the unconditional distribution of the contaminant concentration for any

location and time may be expressed as (References 3, 4, 5, 6):

$$P[C(xyt)] = \iiiint [\, P\{C(xyt) \mid C_L, t_f, K\}\, P\{C_L \mid tf\} \bullet$$
$$P\{t_f \mid p\}\, P\{p\}\, P\{K \mid u_k\}\, P\{u_k \mid v_k\}\, P\{v_k\}\,]\; dC_L\, dt_f\, dp\, dv_k\, du_k$$

where t_f = time to containment failure (or initiation of contamination), C_L = leachate release concentration, K = log hydraulic conductivity field, p = parameter of the distribution, u = mean of the distribution, and v = variance of the distribution. In the deterministic case, the contaminant concentration may be determined conditioned on the specific combination of parameter values chosen. However, in reality, each of the model parameter values may be considered to be a random variable with a specified distribution or a mean, variance and an assumed distribution. In this case, the contaminant concentration must be evaluated as a function of each random variable. Solution of the above integral is intractable, but an alternative is combining probability distributions of input parameters with a deterministic model. Such Monte Carlo simulation experiments were conducted by Medina *et al.* (References 5, 6) with a two dimensional numerical solute transport model. The effect on the probability distribution of the contaminant concentration (at an observation point in the flow field) due to variance in the input parameters, is illustrated in Figure 2. There is only one concentration associated with a probability of 1.0 for the deterministic solution, whereas a spread in the probability distributions represents the uncertainty in the predictions where variability in the input parameters is allowed. Yet, the uncertainty in the predictions is over a much broader range about the deterministic solution for variance in hydraulic conductivity than for variance in time to failure.

A major problem in determining the risks of any site are the uncertainties associated with model parameters such as the leachate release concentration, the hydraulic conductivity field and the time to containment failure. In most cases only mean and variance of the distributions of the individual parameters are known. To incorporate model parameter uncertainties, approximate solution techniques may be used (e.g., Monte-Carlo simulation). An estimate of the cumulative distribution function for the unconditional contaminant concentration is then developed. The unconditional distribution can then be used to assess the risks due to the contamination at any site. Using Bayes' theorem, a more realistic distribution for the contaminant concentrations may be developed conditioned on additional input data. Additional site information concerning any of the model parameters would result in a reduction in the uncertainty of that parameter, which could result in a reduction in the error associated with predicting the groundwater contaminant concentration.

To begin, let the uncertainty associated with the random variable A be defined by the *prior* distribution $P(A)$. The effect of additional information collected through

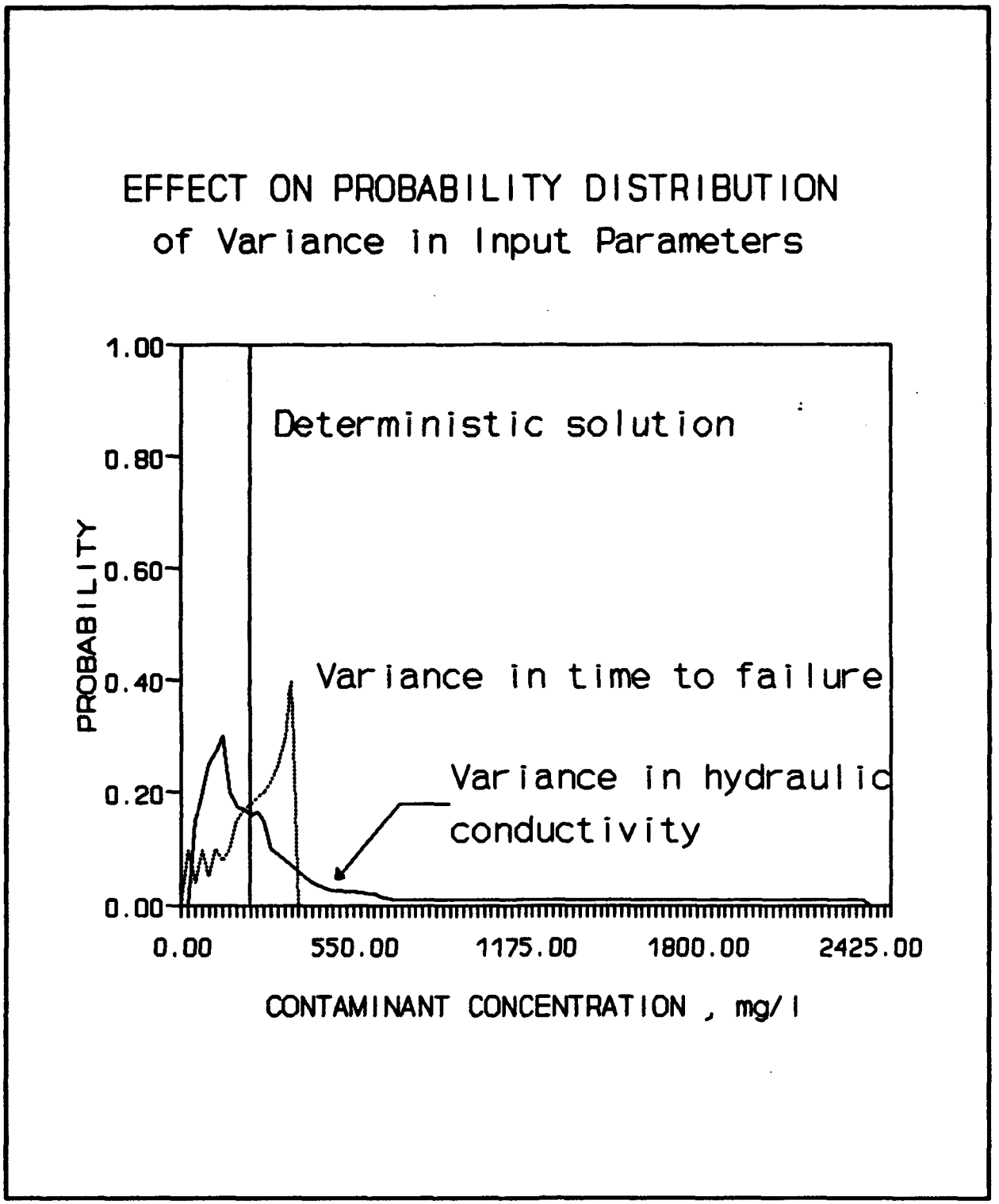


Figure 2. Uncertainty in Subsurface Contaminant Modeling Due to Variance in Input Parameters

field observation and characterized by the conditional probability distribution, $P(I_A|A)$, can now be defined using Bayes' theorem:

$$P(A|I_A) = \frac{P(I_A|A)\ P(A)}{\int P(I_A|A)\ P(A)\ dA}$$

where $P(A|I_A)$ is the updated distribution of the random variable A and is referred to as the *posterior* distribution. The *posterior* distribution reflects the updated distribution of the random variable A.

Bayes' theorem provides an ideal tool for continually assessing the errors and concentrations associated with groundwater contaminant transport. A probabilistic assessment of the groundwater contaminant concentration and its corresponding error can then be used to address the risks associated with a specific site. Regulatory actions or remedial decisions based on this approach can be significantly different and more realistic from those based on a deterministic estimate of groundwater contaminant concentrations when a large amount of variance is present in the unconditional distribution of the contaminant concentration (Reference 6).

This approach has the distinct advantage of being able to more accurately assess the groundwater contaminant concentrations at a specific site. In addition, this methodology allows for the immediate incorporation of new observational data for the site in an effort to further refine the assessment. This decision-making approach could be adapted for Air Force IRP needs.

B. OVERVIEW OF THE ADVISORY SYSTEM

A flow chart illustrating the design of the workstation Advisory System is presented in Figure 3. The user/analyst interacts with a module that controls the flow between the various elements of the system. For example, to the left of the system manager are modules that access stored data (site-specific data, regional data, data on model input parameters) and preliminary screening modules (to rank the severity of contamination at the site under investigation). To the right of the manager module is a transport model selection module, named the CHOICE algorithm, discussed in much greater detail in a later sub-section. It essentially aids the inexperienced user in selection of the solute transport model most appropriate for the site hydrogeology and method of waste disposal. After the appropriate selection is made a plume is predicted and a cumulative probability distribution of contaminant concentration is derived at any desired point in the flow field. The amount of variance in the prediction

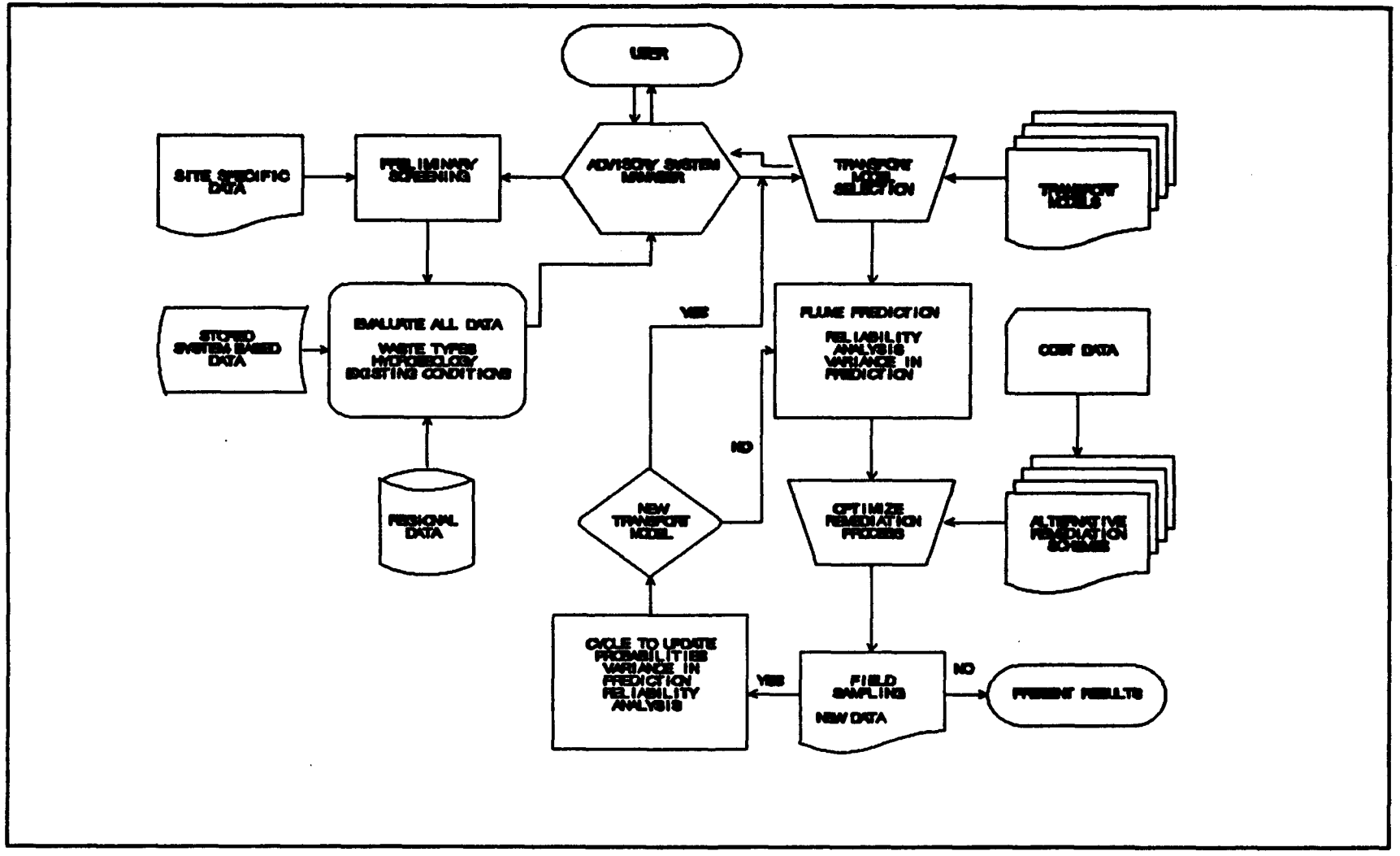


Figure 3. Workstation Advisory System Flow Chart

indicates the degree of uncertainty, which can be reduced by additional field sampling. The next step is optimizing the remediation process, providing a framework for evaluating remediation alternatives and implementing a solution at minimal cost and environmental risk. An algorithm to select remediation alternatives is currently under development. Details of the optimization process are presented below. If further relevant field data is available, the cycle of transport modeling begins again, to possibly reduce the variance in the predictions.

C. OPTIMIZATION OF REMEDIATION

The chance constrained optimization model is multi-objective in nature and driven by probabilistic measures of contaminant concentration in the groundwater surrounding the hazardous waste site. Chance constraints are used to determine the trade-offs that exist between short-term and long-term remediation costs and the probability that the remediation strategy will fail. It is important to emphasize that the whole process depends on the transport models (described in detail below), which are executed in probabilistic mode. The development of an efficient, effective and reliable remediation strategy requires a clear understanding of the site characteristics and the remediation actions implemented. In addition, the optimal remediation strategy must consider trade-offs between the remediation cost and the reliability of the remediation strategy. By investigating these trade-offs, the decision maker can more accurately assess remediation needs, feasible remediation strategies and remediation strategy effectiveness.

Long-term remediation costs will depend on specific remediation considerations and actions. Examples of possible remediation strategies include pulse pumping and treatment, and continuous pumping and treatment. Potential cost savings can be realized by varying the long-term remediation action. The reliability of the long-term remediation strategy represents the likelihood that contaminant concentrations within the groundwater exceeds specified maximums and can be modelled as constraints. These two conflicting goals or objectives can be weighed against one another using a chance constrained optimization model.

Chance constrained modeling is an optimization method in which the physical constraints are originally expressed as probabilistic statements. The technique was first applied to heating oil refinement operations (Reference 7). More recently, chance constrained optimization has been applied in water resources to determine the optimal design and operation of reservoirs conditioned on stochastic streamflows and to manage stream-aquifer systems (References 8, 9, 10). Optimal groundwater remediation strategies are determined by minimizing the long-term and short-term costs associated with the site remediation. In addition, the optimal remediation strategies are conditioned on the probability that the contaminant concentration at any time does not exceed pre-specified maxima. The actual concentrations at any

specified coordinates are calculated by solving the governing differential equations for groundwater contaminant transport, in which key model parameters are expressed as random variables. The resulting optimization model can then be solved using one of several well-established optimization techniques that include Monte Carlo simulation, heuristic search techniques and nonlinear optimization techniques.

Initially, two objectives are being used to drive the optimization model. The first objective is to minimize the long-term remediation costs. One example is the use of waste transport simulation to locate pumping wells, so that contamination concentrations can be lowered below acceptable health standards in the shortest period of time. The second objective will be to maximize the reliability of the long-term remediation strategy by minimizing the probability that contaminant concentrations exceed maximum allowable levels at the site.

Realization of these two objectives will be governed by chance constraints that stipulate acceptable levels of groundwater contaminant concentrations at the hazardous waste monitoring sites. Using the three dimensional form of the solute transport equation for uniform groundwater flow, the model constraint is developed as a probability statement that represents the likelihood of exceeding specified upper bounds on contaminant concentrations. The impact of groundwater treatment and remediation operations are directly incorporated into the governing differential equations for contaminant fate and transport in the groundwater surrounding the site. The general form of the optimization model is:

$$\textit{minimize} \quad Z_1 = COST(\, C(x,y,t))$$

$$\textit{maximize} \quad Z_2 = \max\,\{\alpha\}$$

subject to:

$$P[\, C(x,y,t) \le MCL\,] \ge \alpha \qquad \forall\, x,y,t$$

$$C(x,y,t) \ge 0 \qquad \forall\, x,y,t$$

where $C(x,y,t)$ is the contaminant concentration at any point and time, MCL is the specified maximum allowable contaminant concentration and α is the desired system reliability for any point in the subsurface and time in the planning horizon. Figure 4 presents one possible algorithm for evaluating the chance constrained optimization model.

One major task of solving the optimization model is evaluating the chance constraint. Due to the variability of groundwater parameters and numerical problems associated with solving the governing groundwater equations, the chance constraint

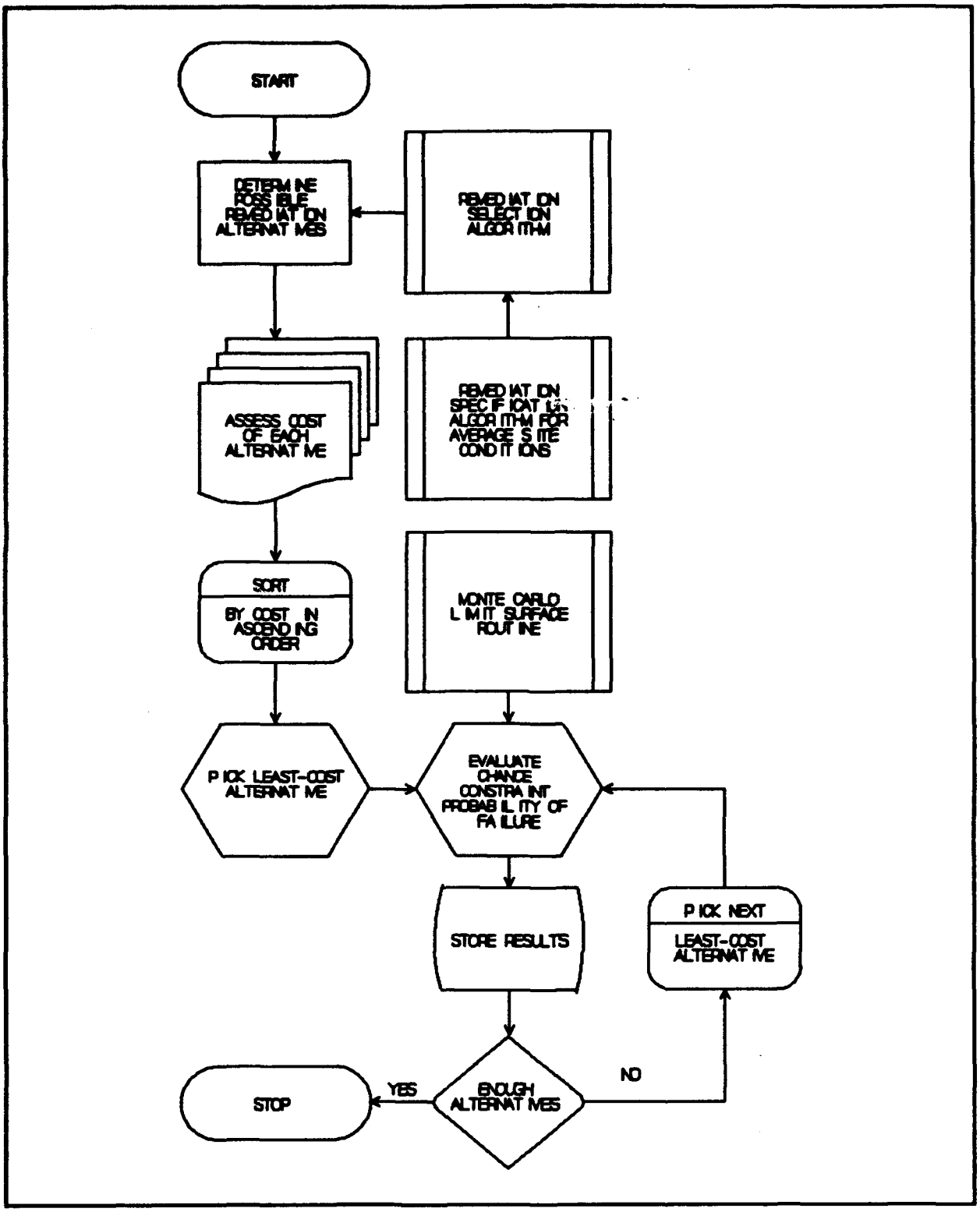


Figure 4. Remediation Optimization Routine

cannot be evaluated directly. One alternative is to use Monte Carlo simulation. However, typical Monte Carlo simulation requires a large number of iterations and can become prohibitive with respect to the required solution time. In addition, data associated with the physical parameters is often lacking for a specific site making it difficult to fully define the probability distributions for important transport properties such as the hydraulic conductivity. To reduce the number of Monte Carlo iterations required while maintaining solution accuracy, a second moment formulation is used to evaluate the chance constraint (Reference 11).

To illustrate the methodology, an example of preliminary results is presented for Operational Unit 3 (OU3) at Hill AFB, Utah in Section III. This example considers only pump and treat activities as a possible remediation strategy. In addition, the hydraulic conductivity, retardation by sorption and porosity are modeled as random variables.

D. COMPONENT MODELS OF THE ADVISORY SYSTEM

1. CHOICE, Algorithm for Model Selection

Ultimately, the management of any system means making decisions aimed at achieving the system's goals without violating specified technical and nontechnical constraints imposed on it (Reference 12). The objective function is to minimize costs and maximize the effectiveness of remediation, which can also be expressed as minimizing the probability of failure. This probability of failure may be defined as the probability of exceeding a regulatory standard.

The nature of the overall modeling process (of which model selection is just one step) may be summarized in five general steps (Reference 13):

- **problem characterization** — the analyst clearly identifies the exposure assessment study objectives and constraints;
- **site characterization** — the analyst reviews all available data, and possibly develops a "conceptual" model;
- **model selection criteria** — the analyst matches the objective, technical and implementation criteria to available models and selects the most appropriate model(s), in this case with the aid of the CHOICE algorithm;
- **code installation** — in the case of a computer code, the model(s) should be properly installed and tested with accepted solutions to standard problems;
- **model application** — the verified model uses site data as input for the contaminant assessment.

CHOICE is not a predictive model, but rather a screening model. The algorithm requests information about the means of waste disposal (e.g., lagoons, landfills, rotary distributors, spray irrigation devices, etc.), the nature of the aquifer, the perimeter of compliance, penetration, type of waste and many other factors. The selection algorithm is part of an interactive, menu-driven management program which executes a large number of supporting decision algorithms and mathematical models. The mathematical details of the models are presented in the next sections, and the theoretical basis of the management modules is presented elsewhere (References 3, 5, 6, 14 and 15). Criteria for choosing among transport models has also been a topic of regulatory interest (References 12 and 13), but without guiding the user to a specific model. The following contaminant transport models have presently been incorporated into the workstation advisory system:

a. Analytical Models
   i. One-Dimensional Transport Model **ODAST** (Reference 16).
   ii. Two-Dimensional Transport Model **TDAST** (Reference 16).
   iii. Two-Dimensional Transport Model **PLUM2D** (Reference 17).
   iv. Two-Dimensional (x,z) Transport Model **DUPVG** (Reference 18).
   v. Three-Dimensional EPA Monte Carlo Transport Model **EPAGW** (Reference 19).
   vi. EPA Monte Carlo Transport Model for Impact on Surface Waters **EPASF** (Reference 20).
   vii. Two-Dimensional Radial Transport Model **LTIRD** (Reference 16).

b. Semi-analytical Model
   i. Two-Dimensional Complex Velocity Potential Model **RESSQ** (Reference 16).

c. Numerical Models
   i. Method of Characteristics Model **MOC** (References 21, 22 and 23).
   ii. Random Walk Solute Transport Model **RWALK** (Reference 24).

Several investigators have compared the performance of numerical codes to analytical solutions, benchmark data sets and real site applications (References 25, 26, 27, 28 and 29). The algorithm for choosing among the numerical codes is based in part on such comparisons. Another version of the algorithm is under development, capable of selection of transport models used to predict the effectiveness of alternative remediation schemes, optimizing for cost/effectiveness. In essence, the first algorithm suggests a model or models for the initial transport prediction: the second will provide guidance on the remediation method, and this may in turn require

selection of another transport code.

The algorithm is outlined in Figure 5. The user responds to screen queries about whether analytical solutions are known to be appropriate or inappropriate (in the latter case, whether the region modeled is homogeneous or heterogeneous). If the complexities require a numerical model, the algorithm then jumps to that branch to select between the two available numerical codes. The flow charts identify the model recommended as a result of certain user responses: whether the subsurface waste disposal method is a landfill, a wastewater lagoon or spray irrigation; whether the flow is radial or not, whether the Dupuit approximation is valid or not; whether single or multiple sources are involved; whether full penetration analysis is adequate; whether regional flow is important or not. For example, the algorithm checks if a particular solution applies: if the user responds in the affirmative that flow in the region is strongly affected by pumping wells, then semi-analytical (complex velocity potential) methods or complete numerical methods would be indicated as more appropriate than models based upon analytical solutions. In the case of selecting a numerical model, the user is prompted to respond to queries about grid size, longitudinal and transverse dispersion, whether the flow is parallel to the grid axes, whether storativity is significant, and whether any part of the aquifer changes from confined to unconfined flow or vice versa.

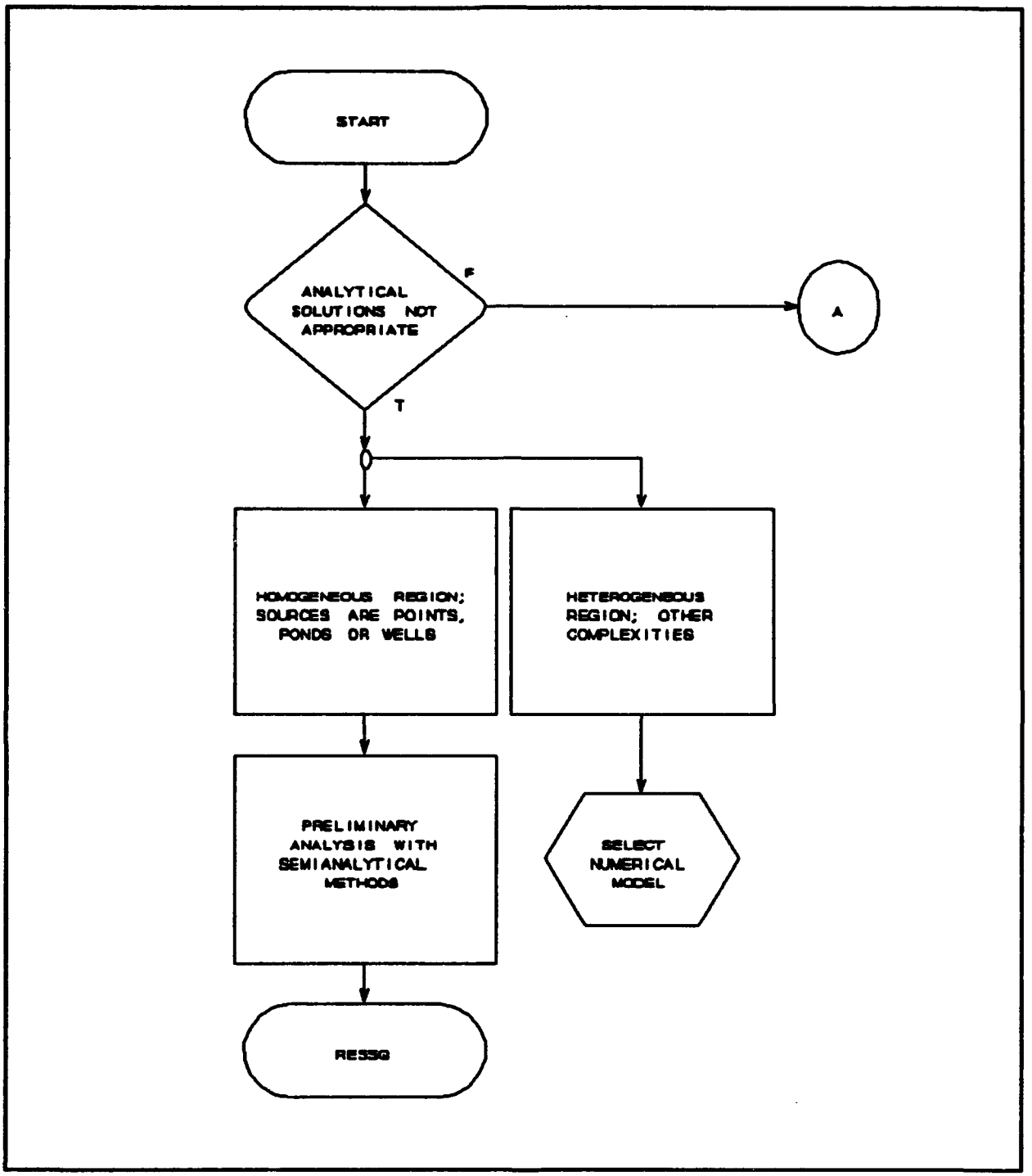


Figure 5. CHOICE Algorithm Flow Chart

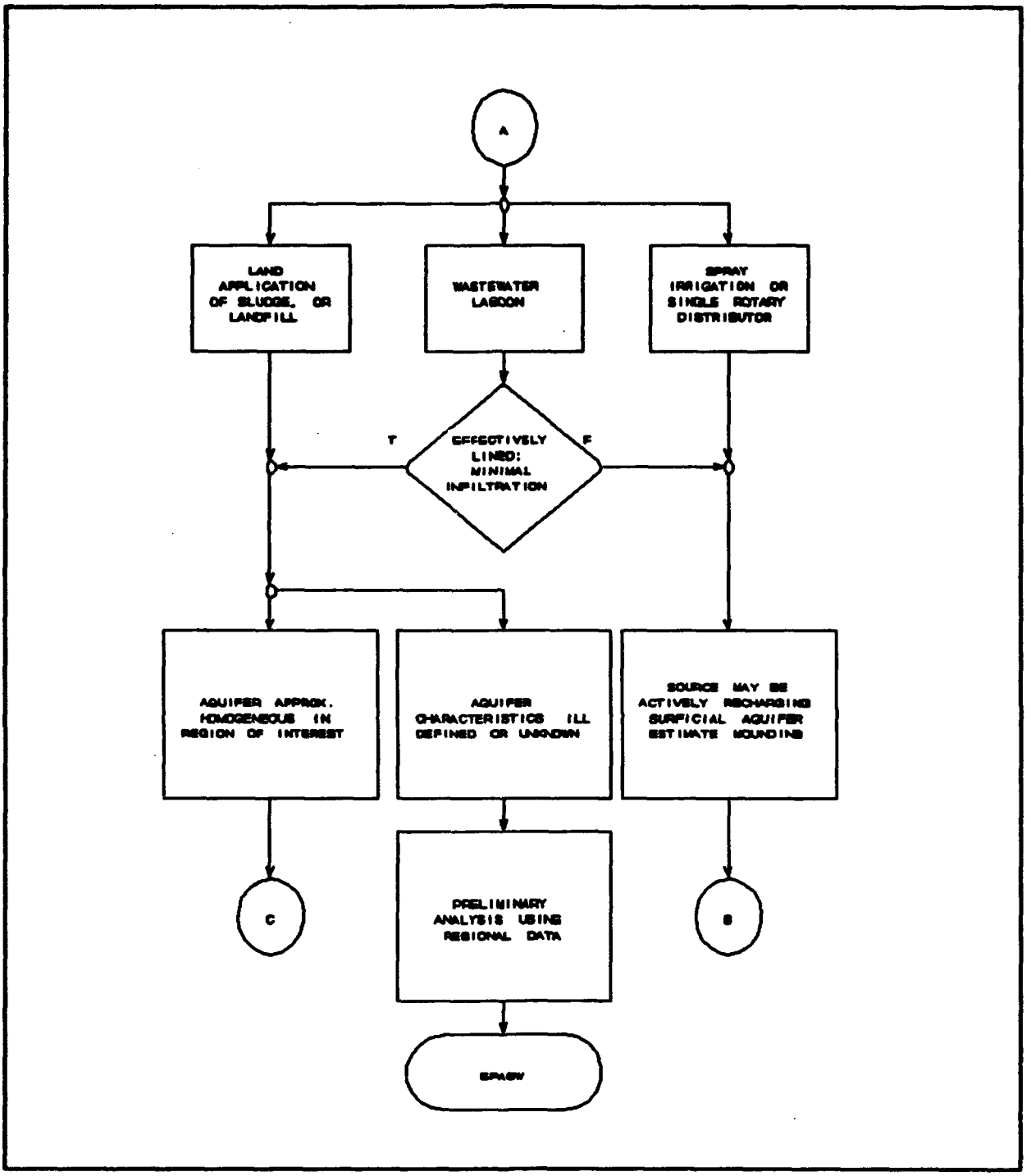


Figure 5. CHOICE Algorithm Flow Chart (cont'd)

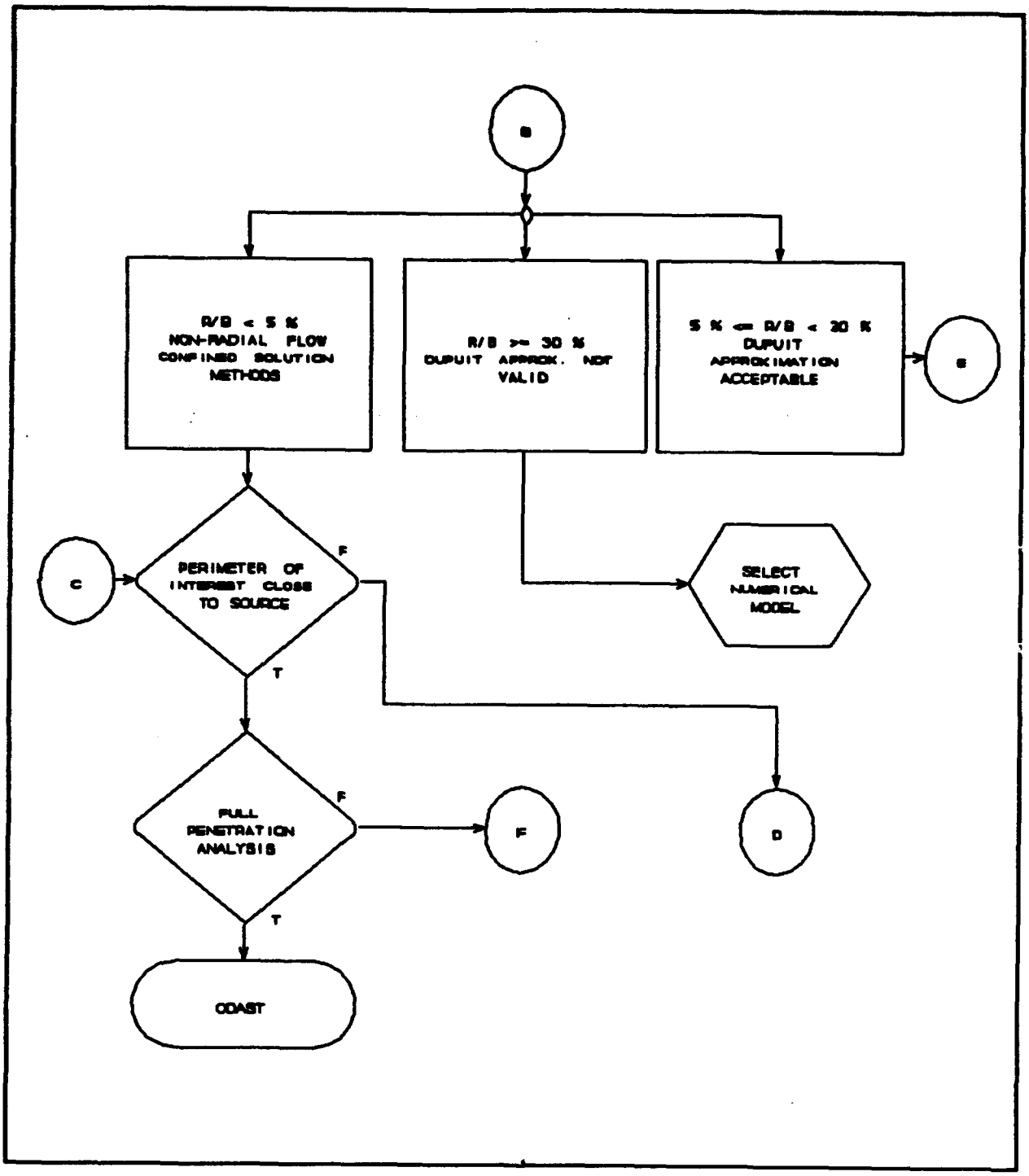


Figure 5. CHOICE Algorithm Flow Chart (cont'd)

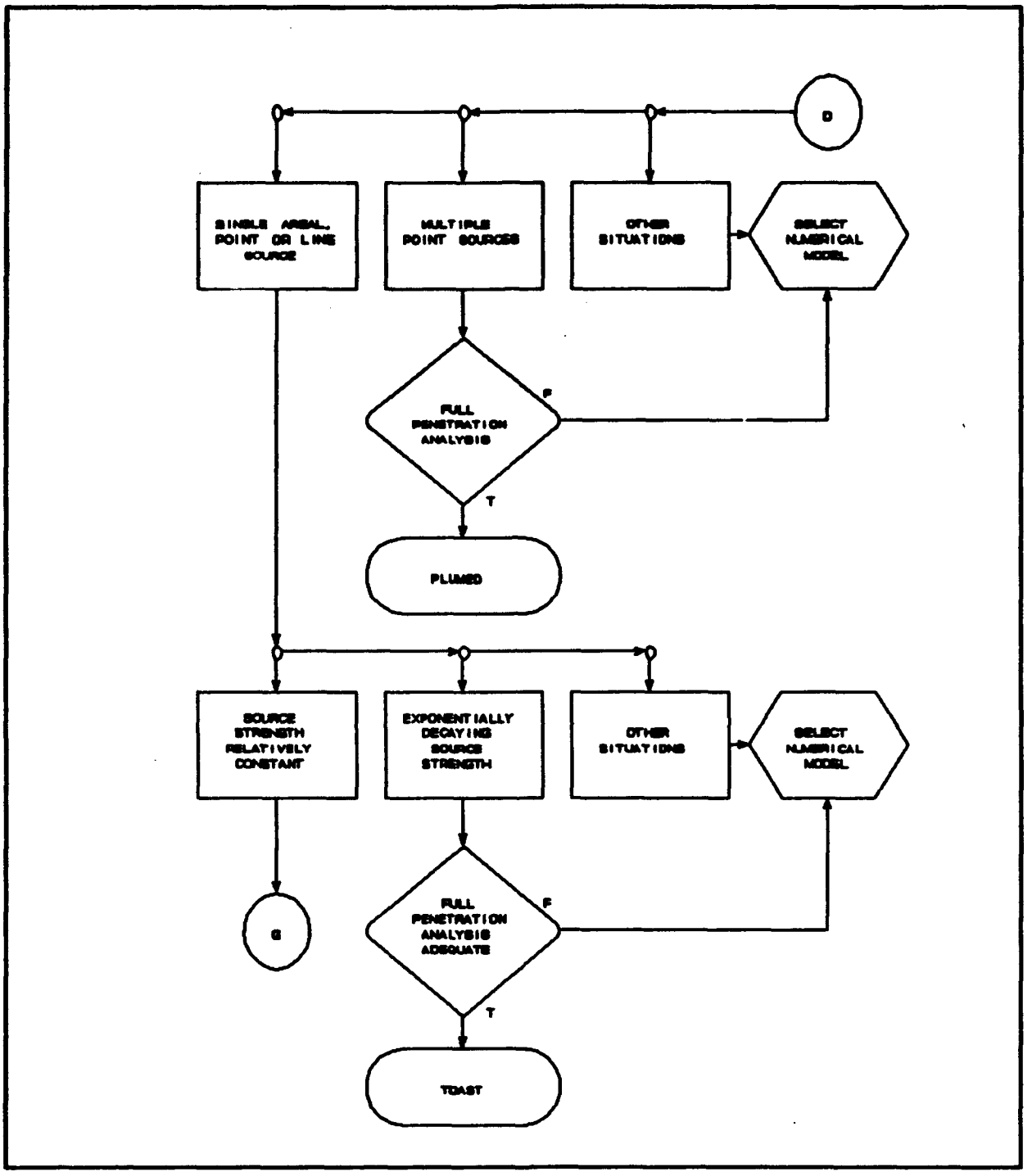
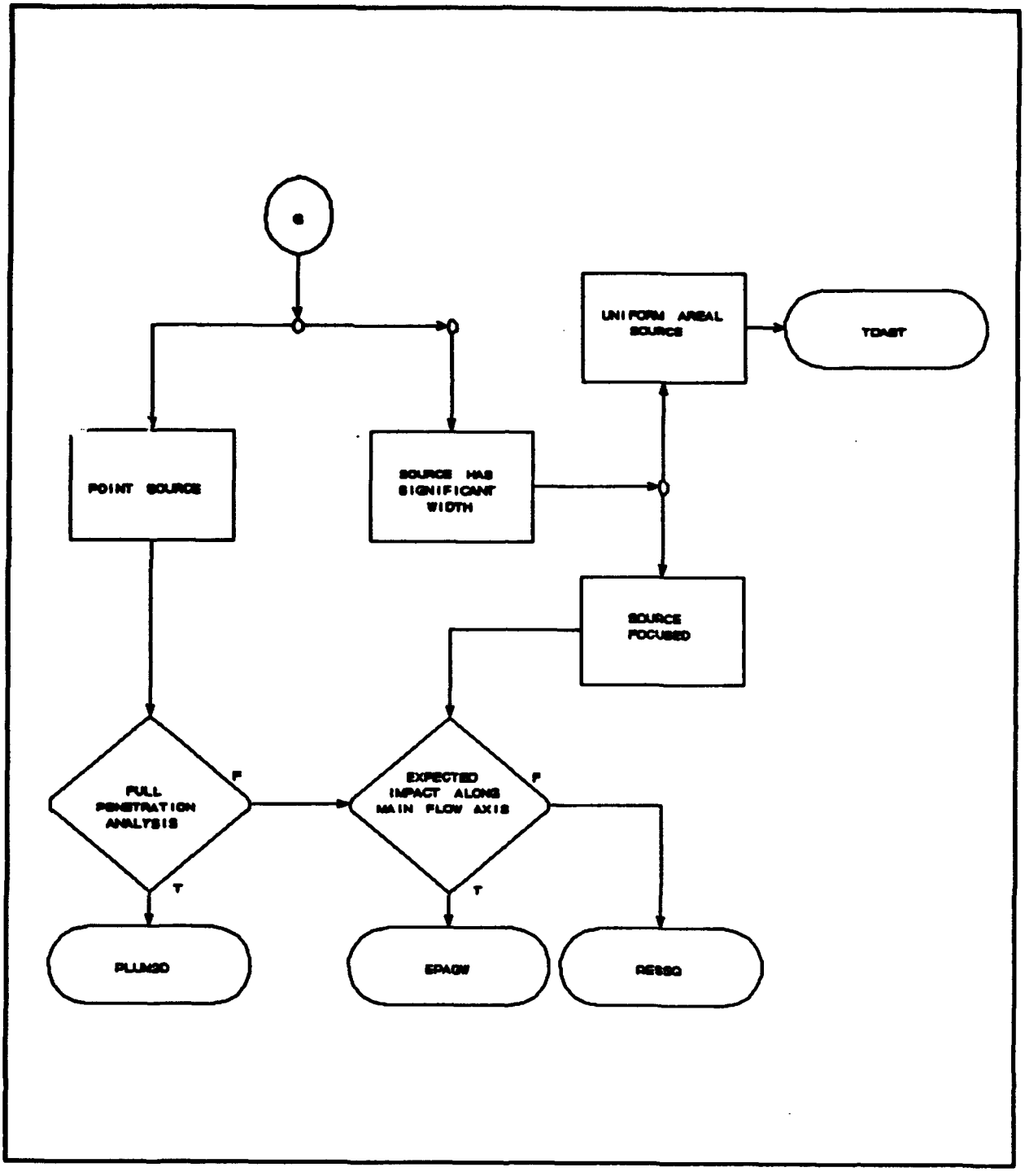


Figure 5. CHOICE Algorithm Flow Chart (cont'd)



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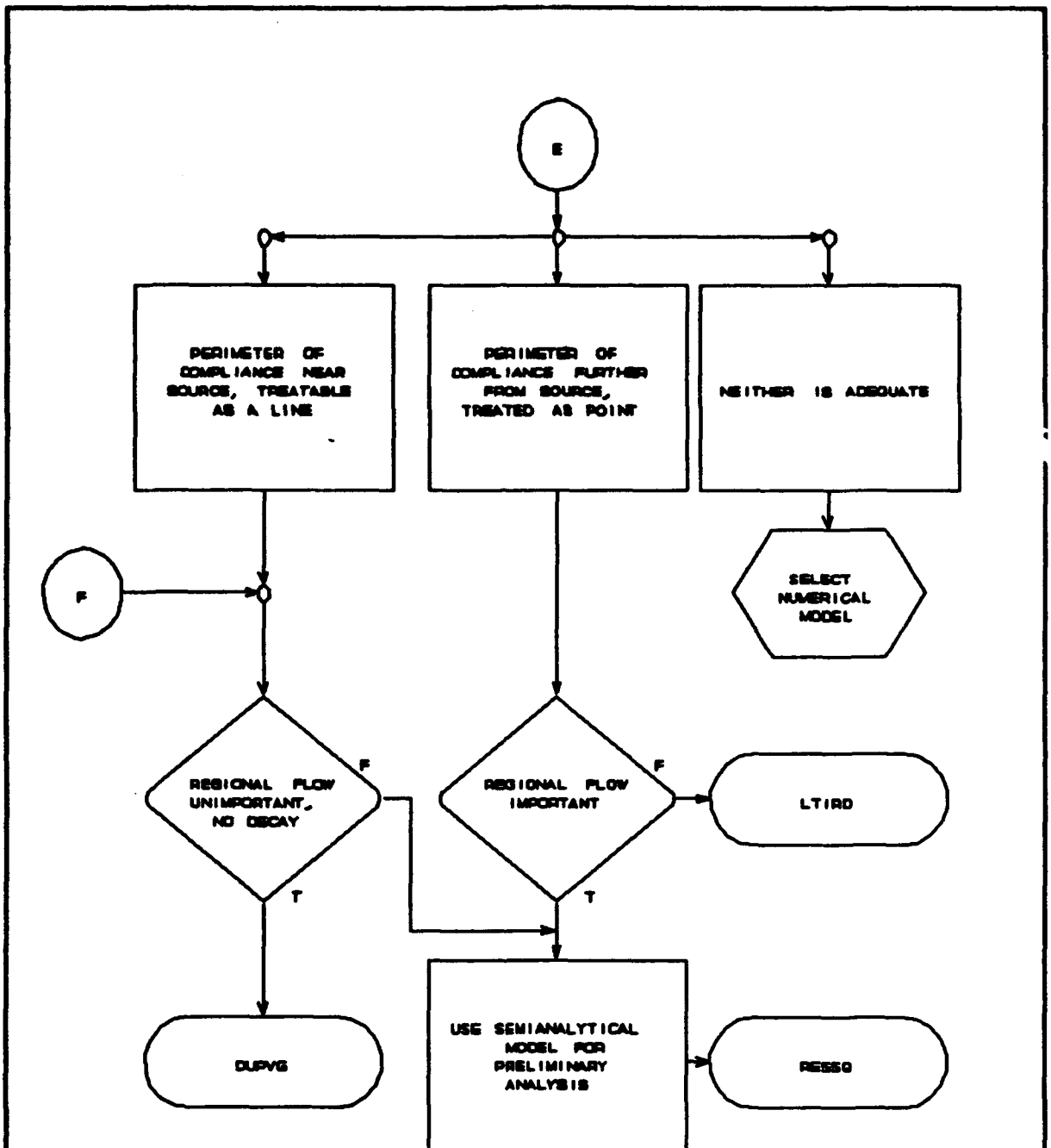

Figure 5. CHOICE Algorithm Flow Chart (cont'd)

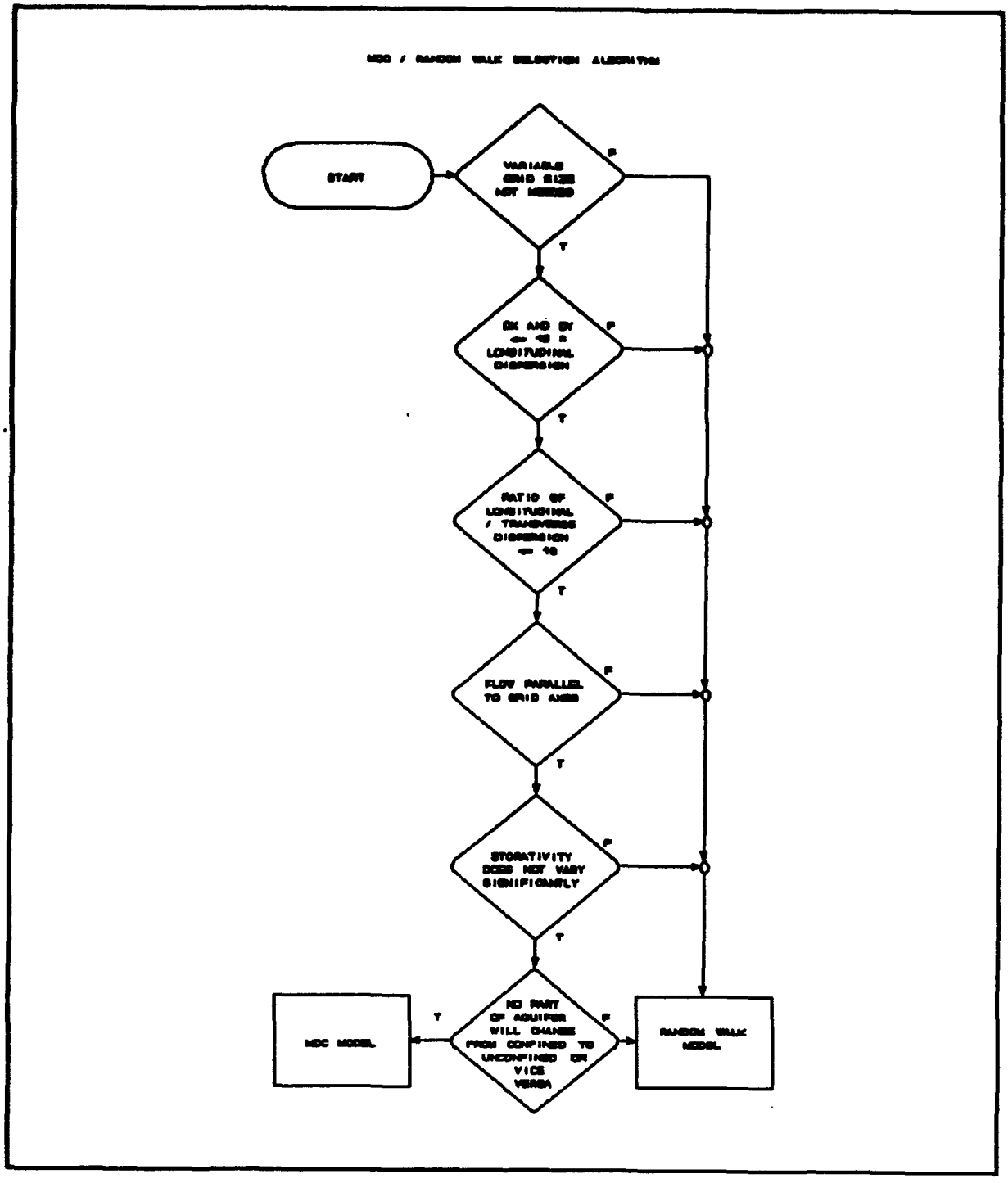

Figure 5. CHOICE Algorithm Flow Chart (cont'd)

2. LeGrand Method

For the purposes of preliminary site analysis, we have included in the System the standardized evaluation methodology developed by LeGrand (Reference 30). The LeGrand method is not a contaminant transport model, but is a tool for the preliminary assessment of a site given certain commonly available information on the site and its environment. The methodology offers a concise screening mechanism for evaluating the contamination potential of waste sites, as well as a management control procedure useful during planning and operational stages of contaminant handling. It is not as comprehensive as the Air Force Automated Defense Priority Model (ADPM).

The LeGrand method focuses on weighting appropriately the key characteristics of a site, in a standardized manner to form a preliminary evaluation of contamination potential. Each key characteristic is assigned a numerical value. The method relies on the quantification of certain parameters, evaluated in a logical sequence, with the results presented in a standardized form. The numerical rating system is divided into ten steps within four stages:

- Standard hydrogeological description of the site. (Stage I)
- Determination of how serious the hazard potential is by identifying the degree of aquifer sensitivity and the degree of contaminant severity. (Stage II)
- Description of the relative probability of contamination by comparing the site's numerical value with a standard value that is derived from consideration of both aquifer sensitivity and contaminant severity. (Stage III)
- Reassessment of the site, with consideration given to engineering modifications. (Stage IV)

Stage I: Numerical Description of Site Hydrogeology

The numerical rating system first provides a description of the site hydrogeology. This is based primarily on four key characteristics:

a. Distance on the ground from a source of contamination to the nearest well, surface stream or property boundary;

b. Depth of the water table below the waste or contamination source;

c. Approximate slope of the water table; and

d. Character of the soil materials through which the contaminant is likely to pass, expressed in terms of permeability and sorption. The method to describe site hydrogeology assigns a "0" value to the most favorable setting of each hydrogeological factor, and a "9" value to the least favorable. Intermediate numerical values are defined by interpolating conditions between the two extremes. For each site the estimated numerical or point value for each of the four factors is added and the total expressed as a number between 0 and 32 that characterizes the site.

This stage consists of seven steps. The first four steps involve the recording of estimated values for each of the four key hydrogeological parameters. These four steps represent the core of the description method.

1. Distance. A great distance between a contamination source and a water supply (or perimeter of regulatory compliance) is generally considered a favorable factor, especially in loose, granular materials with some sorption capacity. It is a less significant factor in fractured materials or cavernous rock, where contamination is likely to reach greater distances. To distinguish one situation from the other the identifying letter T is introduced in Step 6.

2. Depth to the water table. Many contaminants attenuate in the unsaturated zone above the water table. Therefore, it is generally beneficial to have a deep water table. The depth to the water table is defined here as the distance from the ground surface to the surface of water standing in an unpumped well (pumped wells will lower the water table locally). The points assigned increase with shorter distance to the water table. The scale is not a simple arithmetic progression in order to account for the increased sensitivity at smaller depths to the water table.

3. Water table gradient. This factor establishes whether the contaminant is moving toward or away from the water supply (or perimeter of interest). Since the exact gradient is difficult to estimate unless current water table maps are available, only 5 points are spread across this scale.

4. Permeability and sorption. The scale for the permeability-sorption factor extends from 0, representing the low permeability and high sorption characteristic of clay, to 9, representing the high permeability and low sorption of clean gravel. The sites are also classified using a letter qualifier. The letter attached to each digit in the matrix of permeability-sorption is for specific identification of the characteristics of a site.

5. Steps 5 and 6 provide for the addition of letter identifiers that identify special features with respect to the site.

6. In Step 7 the separate ratings and identifying letter suffixes are recorded and the values are added to achieve a total description.

A site description from the LeGrand method is a compound of four separate digits, representing values from the first four steps, and four or more letters derived from Steps 4, 5 and 6. The first letter identifier is derived from the permeability sorption matrix (Step 4). The second letter (A, B or C) assigns a level of confidence to the overall values derived from Steps 1 to 4 (Step 5). The third letter indicates whether the distance from a contamination source is to a well, spring, perennial stream or specified boundary. The fourth letter identifier is selected from the most appropriate characteristic listed with the letter identifiers in Step 6; an additional letter identifier from this list may also be added.

Step 7 completes the site numerical description. It is accomplished by adding the separate point values determined in the first four steps and writing the sum with the appropriate number value and letter suffixes. At this stage the site can be rated in terms of relative hydrogeological conditions, but not necessarily with respect to the possibility of contamination. The site is assigned a grade based on its critical hydrogeological parameters as assessed in Steps 1-6.

Stage II: Evaluation of Degree of Seriousness

The total hazard potential has two components: degree of seriousness and probability of contamination. The degree of seriousness is somewhat independent of the site description obtained in Stage I, but is an essential part of any groundwater contamination evaluation. The analysis performed at this level is made with a matrix considering the sensitivity of the aquifer to contamination and the severity of the contaminant. These factors are defined as follows:

a. Aquifer sensitivity. This term is used to indicate likelihood and degree of groundwater contamination at a given site. The aquifer's areal extent and importance as a ground water source are also considered in this definition. For use in this rating system, aquifers are divided into three categories: sensitive, moderately sensitive and insensitive. Permeability is the key factor in considering aquifer sensitivity. Additional factors are the thickness of the saturated part of the aquifer and the quality of water with respect to its acceptability for use.

b. Contaminant severity. This term includes qualitative weighting of toxicity, concentration and volume, mobility in the groundwater and persistence. The contaminant severity scale ranges from the effluent of a single septic tank at the low end to large volumes of high-level radioactive wastes at the high end.

The overall degree of seriousness is determined by the intersection between

"contaminant severity" and "aquifer sensitivity." The overall degree of seriousness is divided into nine categories, ranging from "relatively small" to "extremely high."

Stage III: Evaluation of Probability of Contamination

The matrix of contaminant severity and aquifer sensitivity is used again in Stage III to grade a situation more specifically. For each intersection of these two parameters a standard situation rating is defined. The standard situation rating represents the approximate numerical value which a site's description should not exceed to prevent serious contamination of groundwater. These PAR values (Protection of Aquifer Ratings) were derived from extensive studies of a large number of situations of varying aquifer sensitivities and contaminant severities, including cases where contamination has or has not occurred. These values, empirical in nature, are then compared with the hydrogeological numerical grade for the site obtained in Stage I. Based on this comparison we obtain a situation rating, from which the probability of contamination, degree of acceptability and situation grade are derived for the site under consideration. Stage III consists of Steps 8 and 9. Step 8 evaluates the probability of contamination and degree of acceptability for a natural site, and Step 9 performs this evaluation for a modified site.

Stage IV: Engineering Improvements and Final Acceptance

Generally, the areas around potential contaminant sites are heavily influenced by human modifications which result in changes in the subsurface hydrologic regime. Engineering modifications to limit contamination are common and should be evaluated. Stage IV provides a means to rate sites that are modified by human action. These changes result in aquifer sensitivity and/or contaminant severity modifications. In Stage IV the effect of the modified properties is reassessed and the new PAR values are evaluated. This results in a new situation rating, giving new probability of contamination, degree of acceptability and situation grade. This stage provides a simple method to predict the impact of human action on the contamination potential of a site, and establish a preliminary evaluation of the cost/benefit ratio.

3. ODAST

The model, ODAST, documented in Javandel et al. (Reference 16), provides an analytical solution of the one-dimensional convective-dispersive transport equation, and is adapted from the set of one-dimensional solutions published by Van Genuchten and Alves (Reference 31).

For the derivation of the model, consider a one-dimensional system

approximated as an infinitely long homogeneous isotropic porous medium with a steady state uniform flow, with seepage velocity v. A dissolved constituent is injected at one end of the model for a period of time t_0, such that the input varies as an exponential function of time. The governing equation for this situation, in a confined homogeneous isotropic aquifer (ignoring the dependence of dispersion on space and time), is:

$$D \frac{\partial^2 C}{\partial x^2} - v \frac{\partial C}{\partial x} - \lambda RC = R \frac{\partial C}{\partial t}$$

where D is the dispersion coefficient, lambda (λ) is a radioactive decay constant, and R is the retardation coefficient. This equation is solved subject to the following initial and boundary conditions:

$$C(x, t) = 0 \qquad t = 0$$

$$\frac{\partial C(x, t)}{\partial x} = 0 \qquad x = \infty$$

$$\left[- D \frac{\partial C}{\partial x} + vC \right] \Big|_{x=0} = v f(t)$$

$$f(t) = c_0 \exp(-\alpha t) \qquad 0 \le t \le t_0$$

$$f(t) = 0 \qquad t > t_0$$

where C_0 and α are constants.

Using the Laplace transform technique, Van Genuchten and Alves (Reference 31) solved this set of equations, obtaining:

$$C(x, t) = A(x, t) \qquad 0 \le t \le t_0$$

$$c(x, t) = A(x, t) - A(x, t - t_0) \exp(-\alpha t_0) \qquad t > t_0$$

where:

$$A(x,t) = C_0 \exp(-\alpha)\ A_1(x,t) \qquad a \neq \lambda$$

$$A(x,t) = C_0 \exp(-\alpha t)\ A_2(x,t) \qquad a = \lambda$$

$$A_1(x,t) = \frac{v}{v+U} \exp\left[\frac{x(v-U)}{2D}\right] erfc\left[\frac{Rx-Ut}{2\sqrt{DRt}}\right]$$

$$+ \frac{v}{v-U} \exp\left[\frac{x(v+U)}{2D}\right] erfc\left[\frac{Rx+Ut}{2\sqrt{DRt}}\right]$$

$$+ \frac{v^2}{2DR(\lambda-\alpha)} exp\left[\frac{vx}{D} + (\alpha-\lambda)\,t\right] erfc\left[\frac{Rx+vt}{2\sqrt{DRt}}\right]$$

$$U = \sqrt{v^2 + 4DR(\lambda-\alpha)}$$

$$A_2(x,t) = \frac{1}{2} erfc\left[\frac{Rx-vt}{2\sqrt{DRt}}\right] + \sqrt{\frac{v^2 t}{\pi DR}} \exp\left[-\frac{(Rx-vt)^2}{4DRt}\right]$$

$$- \frac{1}{2}\left[1 + \frac{vx}{D} + \frac{v^2 t}{DR}\right] \exp\left[\frac{vx}{D}\right] erfc\left[\frac{Rx+vt}{2\sqrt{DRt}}\right]$$

The model can then be adapted for Monte Carlo simulation by treating D and v as random variables. The velocity (v) is not, however, directly generated: it is assumed to result, via Darcy's law, from hydraulic gradient, porosity and hydraulic conductivity. Hydraulic conductivity may be generated directly for the simulation via a log-normal probability distribution. However, this method does not take into account the known relationship between the hydraulic conductivity and other parameters. Therefore, the option is also provided in the code to generate a distribution of hydraulic conductivities from the underlying variables of mean particle size and porosity, from the Karmen-Cozeny relationship. This is the approach most appropriate for preliminary analysis of contamination risk when there is considerable uncertainty regarding the hydrogeology. The underlying variables of gradient and mean particle size are generated for Monte Carlo simulation in the manner described for the model EPAGW.

4. TDAST

The model TDAST provides an analytical solution to steady state flow in a two-dimensional Cartesian coordinate system, and is documented in Javandel et al. (Reference 16) If the flow is coincident with the x axis, and the longitudinal and transverse components of the dispersion tensor are assumed independent of position and designated by D_L and D_T, the general governing equation for a confined, homogeneous, isotropic aquifer can be written as:

$$D_L \frac{\partial^2 C}{\partial x^2} + D_T \frac{\partial^2 C}{\partial y^2} - v \frac{\partial C}{\partial x} - \lambda RC = \frac{\partial C}{\partial t}$$

where lambda (λ) represents decay and R is the retardation coefficient.

For a particular solution, we first assume that the medium is initially free of the solute and that, at a certain time, a strip type source of length 2a, orthogonal to the flow direction, is introduced along the y axis. If the source concentration diminishes exponentially with time, the initial and boundary conditions are:

$$C(o, y, t) = C_0 e^{-\alpha t} \qquad -a \le y \le a$$

$$C(o, y, t) = 0 \qquad |y| > a$$

$$\lim_{y \to \pm\infty} \frac{\partial C}{\partial y} = 0$$

$$\lim_{x \to \infty} \frac{\partial C}{\partial x} = 0$$

Where the source "strip" is arranged orthogonal to the direction of flow, an analytical solution is presented by Cleary and Ungs (Reference 32) as:

$$C(x, y, t) = C_0 \frac{x}{4\sqrt{\pi D_L}} \exp\left[\frac{vx}{2D_L} - \alpha t\right] \cdot \int_{t/R}^{0} \exp\left[-\left(\lambda R - \alpha R + \frac{v^2}{4D_L}\right)\tau - \frac{x^2}{4D_L\tau}\right] \tau^{-3/2} \cdot \left[\operatorname{erf}\left(\frac{a-y}{2\sqrt{D_T\tau}}\right) + \operatorname{erf}\left(\frac{a+y}{2\sqrt{D_T\tau}}\right)\right] d\tau$$

This model can be adapted for Monte Carlo simulation in a manner analogous

to ODAST, except that here the variable D_T must also be generated.

5. PLUM2D

The model we refer to as PLUM2D, originally PLUME 2D, was developed to provide an analytical solution for multiple, fully penetrating point sources in a homogeneous, nonleaky confined aquifer with uniform regional flow, with the flow coincident with the x axis. The solution is documented in van der Heijde (Reference 17). Sources are conceived as fully penetrating wells. In this case, the general governing equation for a solute subject to radioactive decay and adsorption described by a linear, equilibrium relationship can be written as:

$$R_d \frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} - \bar{V} \frac{\partial C}{\partial x} - \lambda R_d C$$

where the dispersion coefficients may be written as:

$$D_x = \alpha_x \bar{V} \; ; \quad D_y = \alpha_y \bar{V}$$

$$\textit{where} \quad \bar{V} = \frac{v}{n}$$

where v is the Darcy velocity, n is the porosity, α_x and α_y are the dispersivity in the x and y direction, R_d is the retardation coefficient, and $\lambda = ln2/T$, with T being the half-life time.

For an infinite two-dimensional porous medium in the x,y plane, with a mass per unit length in the z-direction, M_2, instantaneously injected along the vertical z-axis, the solution is given by:

$$C(x, y, t) = \frac{M_2}{4\pi n t \sqrt{D_x D_y}} \exp \left[- \frac{\left(x - \frac{\bar{V}t}{R_d} \right)^2}{4 D_x \frac{t}{R_d}} - \frac{y^2}{4 D_y \frac{t}{R_d}} - \lambda t \right]$$

The solution may be written by analogy to Hantush's leaky-well function, $W(u,r/B)$, following Wilson and Miller (Reference 33), as:

$$C(x, y, t) = \frac{f_2 \exp\left(\frac{x}{B}\right)}{4\pi n \sqrt{D_x D_y}} W\left(u, \frac{r}{B}\right)$$

where variable B forms the mixing scale equivalent of the Hantush leakage factor, which accounts for the effects of dispersion in the solute transport model.

$$B = \frac{2 D_x}{V}$$

$$r = \sqrt{\left(x^2 + \frac{D_x}{D_y} y^2 \right) \gamma}$$

$$\gamma = 1 + \frac{2B\lambda R_d}{V}$$

$$u = \frac{R^2 R_d}{4 \gamma D_x t}$$

$$W\left(u, \frac{r}{B} \right) = \int_u^\infty \frac{1}{\theta} \exp\left[- \left(\theta + \frac{r^2}{4B^2\theta} \right) \right] d\theta$$

Because of the nature of the solution, various sources may now be superimposed to estimate the result of contamination from multiple point sources, which may have been operational for varying lengths of time. The solution used in the program is obtained by use of an accurate analytical approximation of the Hantush leaky-well function, given by Walton (Reference 34). The model may then be adapted for Monte Carlo simulation in a manner similar to that for other analytical solutions derived here.

6. DUPVG

The model denoted as DUPVG in the system was originally developed to address the problem of solute transport in an unconfined aquifer, where the water table surface may be moving in response to input from a source (References 18 and 35). The equations governing flow and transport in the saturated zone of unconfined aquifers are subject to the non-linear moving free-surface boundary. Where the movement of this free surface is a significant component of the flow regime analytical solutions based on the assumption of a confined aquifer are no longer appropriate. The model of Volker and Guvanasen provides an approximate analytical solution for such cases.

Consider a case in which an infinitely long (in y direction) unconfined aquifer is being recharged through an infinitely long recharge basin of width $2L$. A symmetrical setting is assumed, and the aquifer is bounded by a drain of constant head on each side (x direction) at distance B from the center of the recharge basin. The basin is recharging the aquifer at rate P_0. The medium is assumed homogeneous and uniform

with effective porosity Θ_e, hydraulic conductivity K and initial saturated depth a_0. Flow is assumed to arise only as a result of the recharge (R), which results in a spatially varying head-rise of s.

By symmetry, the solution need be sought only in the $x > 0$ segment. The procedure adopted by the authors is first to solve the flow equations, governing the velocity distribution, then apply these to the transport equation. The rise of the free surface above the initial saturated depth, s, is first obtained by applying the Dupuit-Forcheimer assumption. The resulting equation is then linearized under the assumption that $s/a_0 << 1$, which will be true for small infiltration rates. The equation governing flow is then:

$$\frac{Ka_0}{\theta_e}\frac{\partial^2 s}{\partial x^2} = \frac{\partial s}{\partial t} - \frac{R}{\theta_e}$$

subject to boundary conditions:

$$\begin{aligned} s &= 0, && t = 0, \quad 0 \le x \le B \\ \partial s/\partial x &= 0, && x = 0 \\ s &= 0, && x = B \\ R &= P_0, && 0 \le x \le \le L \\ R &= 0, && L \le x \le B \end{aligned}$$

A solution to this equation can be obtained through the eigen-function expansion method, defining the position of the upper boundary of the saturated flow domain. However, it should be noted that the Dupuit-Forcheimer assumption implies a horizontal flow beneath the basin, where a vertical flow component may actually predominate. To obtain a more accurate representation of the flow field the authors first assume that the flow pattern at any time t can be described as a function of the steady state velocity:

$$u_i\,(x, z, t) = u_i\,(x, z, \infty)\; f(t)$$

where $f(t)$ is the scale function dependent on time. The velocity distribution is then sought by transforming the free-surface flow domain to rectangular coordinates:

$$X \equiv x, \qquad Z \equiv \frac{z\, a_0}{s + a_0}$$

Given the assumption that $s/a_0 << 1$, it can be further assumed that the unsteady free surface can be approximately described by a streamline, that streamline

and equipotential functions change little with time, and that further away from the source the velocity is essentially horizontal and its spatial variation is negligible. Based on these assumptions, only the steady-state velocity pattern in the transformed domain need be sought, and the downstream end can be extended to infinity. The flow equation and associated boundary conditions are simplified to:

$$K\left(\frac{\partial^2 h}{\partial X^2} + \frac{\partial^2 h}{\partial Z^2} \right) = 0, \quad 0 \le X \le \infty, \quad 0 \le Z \le a_0$$

$$K \frac{\partial h}{\partial Z} = P_0, \quad 0 \le X \le L, \quad Z = a_0$$

Solutions are then obtained by the Schwarz-Christoffel transformation method in terms of the relationships between X, Z, and the equipotential and stream function, yielding:

$$X = \frac{a_0}{\pi} \ln \{ \sqrt{\xi} + \sqrt{(1+\xi)} \}$$

$$z = \frac{a_0}{\pi} \cos^{-1} \left\{ \frac{\gamma_1}{\cosh \left(\frac{\pi X}{a_0} \right)} \right\}$$

$$\phi = \frac{Q}{\pi} \ln \{ \sqrt{v} + \sqrt{(1+v)} \}$$

$$\psi = \frac{Q}{\pi} \cos^{-1} \left\{ \frac{\lambda_1}{\cosh \left(\frac{\pi \phi}{Q} \right)} \right\}$$

where

$$\gamma_1 = \epsilon_1 \cosh \left(\frac{\pi \phi}{Q} \right) \cos \left(\frac{\pi \psi}{Q} \right) + \epsilon_2$$

$$\gamma_2 = \epsilon_1 \sinh \left(\frac{\pi \phi}{Q} \right) \sin \left(\frac{\pi \psi}{Q} \right)$$

$$\xi = \frac{1}{2} \left\{ (\gamma_2^2 + \gamma_1^2 - 1) + \sqrt{(\gamma_2^2 + \gamma_1^2 - 1)^2 + 4\gamma_2^2 + 4\gamma_2^2} \right\}$$

$$\epsilon_1 = -\frac{1}{2}\left\{1 - \cosh\left(\frac{\pi L}{a_0}\right)\right\}$$

$$\epsilon_2 = -\frac{1}{2}\left\{1 + \cosh\left(\frac{\pi L}{a_0}\right)\right\}$$

$$\lambda_1 = \frac{1}{\epsilon_1}\cosh\left(\frac{\pi X}{a_0}\right)\cos\left(\frac{\pi Z}{a_0}\right) - \epsilon_2/\epsilon_1$$

$$\lambda_2 = \frac{1}{\epsilon_1}\sinh\left(\frac{\pi X}{a_0}\right)\sin\left(\frac{\pi Z}{a_0}\right)$$

$$\nu = \frac{1}{2}\left\{(\lambda_2^2 + \lambda_1^2 - 1) + \sqrt{(\lambda_2^2 + \lambda_1^2 - 2 + 4\lambda_2^2}\right\}$$

The steady state velocity along streamlines is then given by:

$$\nu(\phi, \psi, t \to \infty) =$$

$$\frac{Q}{\epsilon_1 a_0} \frac{\left[(\gamma_1^2 + \gamma_2^2 - 1)^2 + 4\gamma_2^2\right]^{1/4}}{\sqrt{\cosh^2\left(\frac{\pi\phi}{Q}\right)\sin^2\left(\frac{\pi\psi}{Q}\right) + \sinh^2\left(\frac{\pi\phi}{Q}\right)\cos^2\left(\frac{\pi\psi}{Q}\right)}}$$

By assumption:

$$u_\phi(t) = u_\infty f(t), \quad \text{and}$$

$$f(t) = 1 - \exp\left(\frac{-Ka_0\pi^2}{\phi_e 4B^2}\, t\right)$$

The transformation of the domain is then applied to the transport equation, with the additional transform of time:

$$\tau = \int_0^t f(t)\, d(t)$$

With the assumptions that $s/a_0 << 1$, the slope of the free surface is small, the rate of rise of the free surface is very small, and there is no dispersion across streamlines, the transport equation can be expressed in the curvilinear equipotential-streamline coordinate system as:

$$\frac{\partial C}{\partial \tau} + u_\infty^2 \frac{\partial C}{\partial \phi} = u_\infty^2 \frac{\partial}{\partial \phi}\left(D_L \frac{\partial C}{\partial \phi}\right)$$

For use in the Advisory System we follow Solution S1 as given by Guvanasen and Volker (Reference 35). The reduced governing transport equation is solved subject to the following conditions:

(1) The boundary condition upstream is equivalent to:

$$C(\phi = 0, \tau) = C_0$$

which implies a concentration gradient across the boundary approaching zero.

(2) At the vertical downstream end, with $\phi = \phi_B$:

$$\frac{\partial C}{\partial \phi} = \frac{C}{2D_L}$$

which is an approximation for lower values of C.

(3) The velocity along streamlines at steady state is assumed to be uniform and equivalent to:

$$u_\infty(\phi \rightarrow \infty) = v_\infty = \frac{P_0 L}{(\phi_t a_0)}$$

which assumes that D_L can be taken outside the differentiation, and is thus independent of position.

(4) Initial condition:

$$C(\phi, \tau = 0) = 0.$$

By Laplace transform methods, Volker and Guvanasen (Reference 18) show that the solution then becomes:

$$C(\phi, \tau) = C_0 \exp\left(\frac{\phi}{2D_L}\right) \sum_{n=-\infty}^{\infty} \left(\frac{-1}{2}\right)^n \left(\exp\frac{(-\phi + 2n\phi_B)}{2D_L} \cdot \right.$$

$$\left. \operatorname{erfc}\frac{(\phi - 2n\phi_B - v_\infty^2\tau)}{2v_\infty\sqrt{D_L\tau}} + \exp\left(\frac{\phi - 2n\phi_B}{2D_L}\right) \cdot \operatorname{erfc}\frac{(\phi - 2n\phi_B + v_\infty^2\tau}{2v_\infty\sqrt{D_L\tau}}\right)$$

Noting that B, the distance to the constant head boundary, goes to infinity, a good approximation to the equation above is:

$$C = \frac{C_0}{2}\left\{ erfc\ \frac{(\phi - v_\infty t)}{2v_\infty\sqrt{D_L \tau}} + \exp\left(\frac{\phi}{2D_L}\right) erfc\ \frac{(\phi + v_\infty^2 \tau)}{2v_\infty\sqrt{D_L \tau}} \right\}$$

This approximation will not be particularly good when B is small relative to the distance from the source. However, this approximation is only involved in the solution of the transport equation, and not in the solution of the velocity equation. Thus the error should not affect the computed average position of the front.

7. EPAGW, Modified EPA Model for Monte Carlo Analysis of Impact On Groundwater

This groundwater model accounts for most of the major physical and chemical processes that affect movement and transformations of chemicals in simple, homogeneous and isotropic porous media under steady flow conditions (Reference 20). The mechanisms considered include advection, hydrodynamic dispersion in the longitudinal, lateral and vertical dimensions, adsorption and chemical degradation. Major assumptions made by the transport model are:

a. groundwater velocity is uniform, one-dimensional and steady-state, in a saturated aquifer;

b. the porous medium is homogeneous and isotropic;

c. mass transport is also in a steady state;

d. the aquifer is semi-infinitely large in the direction of groundwater flow and infinitely large in the transverse direction;

e. the contaminant source is sufficiently large in mass such that the down-gradient concentration will be maintained once it is reached;

f. the distribution of contaminant concentration at the source boundary is Gaussian;

g. degradation of chemicals is caused only by hydrolysis;

h. equilibrium, reversible speciation, and sorption are appropriate -- in order to utilize an equilibrium partition coefficient.

The advection-dispersion equation for the transport of a nonconservative contaminant in an adsorbing homogeneous and isotropic porous medium with fully-saturated flow may be written as follows:

$$D_{xx} \frac{\partial^2 C}{\partial x^2} + D_{yy} \frac{\partial^2 C}{\partial y^2} + D_{zz} \frac{\partial^2 C}{\partial z^2} -$$

$$\frac{V}{R_f} \frac{\partial C}{\partial x} = \frac{\partial C}{\partial t} + \lambda C + IC$$

where

x,y,z	=	spatial coordinates in the longitudinal, lateral and vertical directions, respectively, *(L)*;
C	=	dissolved concentration of chemical, (M/L^3);
D_{xx}, D_{yy}, D_{zz}	=	retarded dispersion coefficients in the x,y and z directions, respectively, (L^2/T);
V	=	groundwater seepage velocity, assumed to be in the *x* direction, *(L/T)*;
R_f	=	retardation factor;
t	=	elapsed time, *(T)*;
Θ	=	volumetric water content of the porous medium;
I	=	net recharge due to precipitation, (T^{-1}).

The retardation factor and the effective reaction rate constant are defined as follows:

$$R_f = 1 + \frac{\rho_b K_d}{\theta}$$

$$\lambda = \frac{\lambda_1 \theta + \lambda_2 \rho_b K_d}{\theta + \rho_b K_d}$$

where

ρ_b	=	bulk density of the porous medium, (M/L^3);
K_d	=	distribution coefficient, (L^3/M);
θ	=	volumetric water content;
λ_1	=	rate coefficient for dissolved phase, *(1/T)*;
λ_2	=	rate coefficient for sorbed phase, *(1/T)*.

The three-dimensional region of interest is regarded as semi-infinite in the *x*-direction ($0 \leq x < \infty$), infinite in the *y*-direction ($-\infty < y < \infty$), and finite in the *z*-direction ($0 \leq z \leq B$), where *B* is equal to the saturated zone thickness. The above partial differential equation is solved analytically. The solution treats the source concentration as a Gaussian distribution in the lateral direction (along the *y*-axis corresponding to the leading, down-gradient edge of the unit), and a uniform distribution over the vertical mixing or leachate penetration depth, *H*. The maximum dissolved concentration of contaminant, C_o, occurs at the center of the Gaussian

distribution, y_o. This distribution is defined by its standard deviation, σ, which is measured in terms of distance (in meters) and is related to the width of the disposal unit. The initial and boundary conditions necessary to solve the equation may be written as follows:

$$C(x, y, z, 0) = 0$$

$$C(o, y, z, t) = C_0 \exp(-y^2/2\sigma^2) \; U(Z)$$

$$C(x, \infty, z, t) = 0$$

$$C(x, -\infty, z, t) = 0$$

$$C(\infty, y, z, t) = 0$$

$$\frac{\partial C}{\partial x}(x, y, 0, t) = 0$$

$$\frac{\partial C}{\partial x}(x, y, B, t) = 0$$

where C_0 is the peak concentration at the source, σ is the standard deviation of the Gaussian distribution centered at $x = y = 0$, and $U(z)$ is a unit step function

$$U(z) = 1 \quad , \quad H_1 \le z \le H_2$$
$$U(z) = 0 \quad , \quad z > H_1 \text{ or } z > H_2$$

A steady-state analytical solution can be obtained by direct solution of the steady-state version of the governing differential equation, which implies removal of the time-derivative term. Details of the solution procedure are contained in a U.S. EPA report (Reference 36). The solution is:

$$c_p(x, y, z) = \frac{H}{B} c_f(x, y) + \Delta c_p(x, y, z)$$

where

$$c_f(x, y) = \xi' \int_{-\infty}^{\infty} \frac{\exp(-y_p^2/2\sigma^2)}{\sqrt{x^2 + (y_p - y)^2 D_x/D_y}}$$

$$\cdot K_1 \left\{ \sqrt{\frac{\eta x^2}{D_x} + \frac{\eta (y_p - y)^2}{D_y}} \right\} dy_p$$

and

$$\Delta c_p(x, y, z) = \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{1}{n} \sin\left(\frac{n\pi H}{B}\right) \cos\left(\frac{n\pi z}{B}\right)$$

$$\cdot \xi' \int_{-\infty}^{\infty} \frac{\exp(-y_p/2\sigma^2)}{\sqrt{x^2 + (y_p - y)^2 \frac{D_x}{D_y}}} \cdot K_1 \left\{ \left[\frac{\beta_{nx}^2}{D_x} + \frac{\beta_n (y_p - y)^2}{D_y} \right] \right\} dy_p$$

in which y_p is a dummy variable of integration, and ξ' is a constant:

$$\xi' = \frac{x c_0}{\pi} \sqrt{\frac{B_n}{D_y}} \exp\left(\frac{V_s x}{2D_x}\right)$$

$$\eta = \frac{V_s^2}{4D_x} + \lambda + 1$$

$$\beta_n = n + \frac{n^2 \pi^2 D_z}{B^2}$$

and $K_1(\cdot)$ is the modified Bessel function of the second kind and of first order. The solution given assumes that the source extends from the top of the aquifer through the thickness H, so that $H_1 = 0$ and $H_2 = H$.

To obtain the steady-state concentration distribution along the x (flow) axis, the solution can be reduced to:

$$c_p(x, 0, 0) = \frac{H}{B} c_f(x, 0) + \Delta c_p(x, 0, 0)$$

where:

$$c_f(x, 0) = \xi^* \int_0^{\infty} \exp\left\{ -\left(\frac{\sigma^2 \xi^2}{2} + x \sqrt{\frac{\xi^2 D_y}{D_x} + \frac{n}{D_x}} \right) \right\} d\xi$$

$$\Delta C_p(X,0,0) = \frac{2}{\pi}\sum_{n=1}^{\beta}\frac{1}{n}\sin\left(\frac{n\pi H}{B}\right)\cos\left(\frac{n\pi z}{B}\right)$$

$$\cdot\,\xi^{*}\int_{0}^{\infty}\exp\left\{-\left(\frac{\sigma^2\xi^2}{2}+x\sqrt{\frac{\xi^2 D_y}{D_x}+\frac{B_n}{D_x}}\right)\right\}d\xi$$

$$\xi^{*} = \frac{2c_0\sigma}{\sqrt{2\pi}}\exp\left(\frac{V_s x}{2D_x}\right)$$

El-Kadi *et al.* (Reference 37) applied this model to six waste disposal sites in different regions of the United States. The model was tested against a three-dimensional finite element model (CFEST) and was found to generally underestimate the contaminant concentrations: they recommend using a factor of safety of one order of magnitude for a conservative analysis. It should be emphasized that the "exact" results were taken to be those produced by the numerical model. Overestimation of concentrations resulted when the model was applied to a site where radial flow existed. With appropriate choice of parameters, analytical solutions are especially suitable for management purposes when combined with sensitivity analysis and/or uncertainty analysis (e.g., Monte Carlo simulation).

Input data for all model parameters must be identified to use the EPAGW model. In general, however, the behavior of a specific constituent in the environment is highly dependent on both the environmental setting and the properties of the constituent. The assignment of specific values to describe the behavior of the modeled system is further complicated by uncertainty about how to specify a single value for each model parameter which represents a "worst case" (obtained from the steady-state solution along the *x*-axis).

As an alternative to identifying reasonable worst-case values for each model, a Monte Carlo simulation technique is used. It involves a large number of computer runs with values for each input parameter drawn from data sets describing ranges of possible values and the distribution of values within the range. Where parameters are correlated, and therefore dependent, the relationships are properly defined in the Monte Carlo routine. The Monte Carlo process in EPAGW (and in general) proceeds as follows:

(1) Values from each input distribution are selected at random.
(2) The model is run with a set of randomly-generated parameters to give a set of output variables.
(3) The input selection and computation steps are repeated a large number of times (1000 to 5000) to produce a well-defined output distribution.
(4) The output values are analyzed for presentation as distribution.

The groundwater model parameters and input data requirements include the following: groundwater velocity, porosity of the saturated media, dispersivity of the aquifer, distance to the measurement point, standard deviation of the Gaussian source, penetration depth of leachate into the aquifer, thickness of aquifer, fraction of organic carbon content of the soil, pH and temperature of groundwater, acid, neutral and base hydrolysis rates. Relationships between these environmental parameters must be determined in order to apply the Monte Carlo analysis properly. All the parameters and input data previously mentioned are in some extent linked or dependent on at least one of the others. In some cases an independent seed distribution can be generated to which other variables are correlated. Such is the case of temperature, which is not a function of any of the other parameters, but influences the values of some of them (e.g., hydrolysis rate coefficients). Dependent data sets can be developed as empirical, joint or multivariate distributions, theoretical distributions, or from functional dependencies among the variables and parameters. The parameters and variables to be generated independently are as follows:

a. Thickness of the saturated zone, *B*

b. Fractional organic carbon content, *FOC*. The fractional organic carbon content is used to determine the distribution coefficient, K_D, from the following relationship:

$$KD_D = (f_{oc})\ (K_{oc})$$

where

K_{oc} = distribution coefficient normalized to organic carbon.

c. Groundwater pH, assumed to be independent of contaminant concentration and temperature.

d. Groundwater temperature, *T*.

e. Leachate penetration into the saturated zone, *H*, probably related to the relative differences in the leachate and groundwater velocities. A simple, independent, uniform distribution ranging from a fixed minimum to a fixed maximum is used to represent this variable.

f. Net recharge, *I*. It is the amount of water that enters an aquifer system. Since the groundwater model assumes that the porous media is uniform, the effect of recharge causes the groundwater to rise and fall uniformly. There is thus no change on the gradient or groundwater velocity. *I* is estimated as follows:

$$I = q'/H$$

where q' = net infiltration, *m* / year

H = leachate penetration depth, *m*.

The remaining input parameters and variables are dependent and cannot be generated without properly matching each value with other related values. Dependencies are considered with the objective of avoiding unrealistic or impossible sets of data, that is, to provide consistent sets of data. In general, precise functional relationships among all the dependent variables or parameters do not exist. Similarly, observed data for all values taken in sets do not exist or are inadequate in number to permit statistical representation of these dependencies. However, equations do exist in the engineering and scientific literature to permit generation of sets of possible combinations of input data. The parameters and variables to be generated as dependent values are as follows:

$\alpha_L, \alpha_T, \alpha_V$ = dispersivities in the longitudinal, lateral and vertical directions assumed to be largely dependent on distance, *x*.

Θ = porosity of the soil or porous media, assumed to be largely dependent on soil properties and parent material.

ρ = bulk density of the soil or porous media, largely dependent on soil properties including porosity.

V = groundwater flow velocity, largely dependent on soil properties including hydraulic conductivities, porosity, bulk density and hydraulic gradient.

σ = standard deviation of the gaussian distribution representation of the source concentration, related via mass balance principles to leachate volumes, groundwater velocity, porosity, and depth of leachate penetration into the saturated zone.

K_a, K_n, K_b = hydrolysis rate constants, dependent on groundwater *pH* and temperature, and on specific chemical properties.

K_D = effective distribution coefficient for each specific chemical. It is assumed to be dependent on the organic carbon content of the soil, and in some cases on the *pH* and specific chemical properties of the pollutant.

The relationships used for the generation of these parameters and variables are discussed below.

g. Dispersivity. Guven *et al.* (Reference 38) reported a simple, linear dependency on the travel distance for the longitudinal dispersivity, of the form:

$$\alpha_L = 0.093\,X + 0.007$$

where X = mean travel distance, *m*.

Transverse dispersivity, α_T, has been studied to a lesser degree but its magnitude is known to be less than the longitudinal dispersivity while maintaining scale dependency (Reference 39). Typically, α_T is related to α_L by a simple ratio leading to the expression:

$$\alpha_L / \alpha_T = LTR$$

where LTR = longitudinal/transverse dispersivity ratio.

However, such ratios are often assumed quite arbitrarily. The actual relationship is the subject of current research. A range of LTR has been reported that appears to center around a value of 3.0, which has been selected for the EPAGW Monte Carlo analysis. For multidirectional flow in the longitudinal direction the vertical dispersivity, α_V, is quite low. Using the ratio α_L/α_V to describe vertical dispersivity, Gelhar *et al.* (Reference 40) reported a range of 30 to 1860, with an average of 400. Because of the uncertainty surrounding proper specification of values for vertical dispersivity, it is varied uniformly from 40 to 400 in the Monte Carlo routine.

The data generation approach for dispersivity can be summarized by the following equations:

$$\alpha_L = 0.093 X + 0.007$$

$$\alpha_T = 0.0333 X$$

$$\alpha_V = 0.0025 X - 0.01 X$$

where X is the downgradient exposure point distance selected for the implementation of the decision rule.

h. porosity, Θ. It is the ratio of the volume of voids of a given soil to the total volume of soil. It is largely a function of particle size. For small particle size like clay, porosity increases to a maximum of about 0.5. Porosities of coarse media (e.g. gravel) decrease to a minimum of about 0.3. These measured ranges suggest a strong correlation with mean particle diameter, d. Data reported by Davis (Reference 41) were used to develop a regression equation relating porosity to mean particle size as follows:

$$\Theta = 0.261 - 0.0385 \ln (d)$$

where $\ln (d)$ = natural logarithm of the mean particle diameter.

The distribution for porosity is generated from a seed distribution for particle size diameter. After a uniform and a log-uniform distribution for the particle size diameter were investigated, the log-uniform distribution was selected because it more heavily weights the influence of smaller particle sizes and because the related velocity distribution is more consistent with observed data.

i. Bulk density is defined as the mass of dry soil divided by its total or bulk volume. According to Freeze and Cherry (Reference 42):

$$\theta = 1 - \frac{\rho_b}{\rho_p}$$

where ρ_p = particle size density, g/cm^3 ;

ρ_b = bulk density, g/cm^3.

The particle density of soil materials varies over a very narrow range, with an average 2.65 g/cm^3. Substituting this value in the porosity equation, the bulk density may be calculated as a function of porosity as follows:

$$\rho_b = 2.65 \ (\ 1 - \theta \ )$$

j. Velocity, *V*. The velocity of groundwater is a major determinant of the transport of solutes in subsurface systems. In uniform porous media it is the dominant factor and must be properly specified in the Monte Carlo process. Dependencies among its input data must be preserved while generating realistic values of velocity.

Velocities are related to soil properties and other site-specific factors through Darcy's Law. Assuming steady flow in uniform, saturated media, Darcy's Law states (in simplified form):

$$V = \frac{K_s \ S}{\theta}$$

where K_s = saturated hydraulic conductivity, cm/sec
S = hydraulic gradient.

The saturated hydraulic conductivity is a measure of the ease with which water flows though porous media. For any given fluid, it is a function of the medium properties including particle size, grain shape, connectivity and tortuosity. Several approximate functional relationships to estimate the value of K_s have been proposed. The most notable among them is the Karmen-Cozeny equation (Reference 43):

$$K_s = 478\left(\frac{\theta^2}{(1-\theta)^2} d^2 \right)$$

where Θ = porosity;
d = mean particle diameter.

The hydraulic gradient, S, is a function of the local topography, groundwater recharge volumes and locations, and the influence of withdrawals, and it is indirectly related to porous media properties. Since there is no functional relationship to express these dependencies, another independent seed distribution is required to generate this variable. To prevent unrealistic conditions due to very large values of the velocity caused by high values of both K_s and S, the velocity field may be bounded such that a fixed maximum is not exceeded.

k. Standard deviation of the Gaussian distribution for the source concentration, σ. This parameter reflects the nature and extent of the leachate interaction with the groundwater. From mass balance principles it may be stated that

$$\sigma = \frac{q A_w C_L}{\sqrt{2\pi}\ V\theta\ H C_o}$$

where

q = unit areal flux of leachate through the land disposal facility, m / year;
A_w = area of disposal facility, m^2;
V = groundwater velocity, m /year;
Θ = saturated zone porosity;
H = leachate penetration into the saturated zone, m;
C_L = contaminant concentration in the leachate;
C_o = contaminant concentration in the mixing zone beneath the facility.

Assuming that the leachate concentration is the same as the maximum concentration of the Gaussian concentration distribution, σ can be calculated directly from the equation above given the other variables. This assumption implies that the leachate displaces the groundwater and dilution begins after advective transport has been initiated. Values for the chemical flux, q, and the area term, A_w, were generated by independent seed distributions. For mathematical reasons (boundary effects) the constraint that the ratio H/B be less than 0.5 must also be made. The minimum saturated thickness is set to 3 meters.

l. Hydrolysis rates. Hydrolysis rates depend on the chemical nature of the pollutant and have to be taken from the literature or measured experimentally in the laboratory. Acid and base-catalyzed hydrolysis rates depend on groundwater pH, and acid, base and neutral hydrolysis rates are a function of temperature. The temperature dependency has been described using the Arrhenius equation. Using the generic activation energy recommended by Wolfe (Reference 44) of 20 kcal/mole, the temperature correction factor can be written as :

$$K^{T}_{a,n,b} = \exp\left[10^{4}\left(\frac{1}{T_r} - \frac{1}{T}\right)\right]$$

where

$K^{T}_{a,n,b}$	=	second-order hydrolysis rate constant for acid, neutral, or base conditions at temperature T;
$K^{Tr}_{a,n,b}$	=	second-order hydrolysis rate constant for acid neutral or base conditions at reference temperature T_r;
T	=	temperature, °K;
T_r	=	reference temperature, °K.

m. Distribution Coefficient. In most cases, the sorption process is dominated by hydrophobic binding. It is possible then to relate the distribution coefficient directly to the soil organic carbon. As stated earlier, the dependency is given by:

$$k_D = (k_{oc})\ (f_{oc})$$

where

k_{oc}	=	distribution coefficient normalized to organic carbon;
f_{oc}	=	fractional organic carbon.

The values for fractional organic carbon are generated as an independent parameter. For other binding mechanisms, as those presented by polar or ionizable compounds, adjustments are made on a case-by-case basis (Reference 45). In cases where reliable relationships do not exist, measurements are required.

8. EPASF, Modified EPA Model For Analysis Of Impact On Surface Water

As part of rules for land disposal restrictions proposed by the U.S. Environmental Protection Agency (Reference 20), models were developed for the back-calculation of screening levels of constituents in land disposal systems under conditions of uncertainty. The models developed for this purpose considered the impacts of hazardous constituents both in groundwater and in surface waters contaminated via migration through groundwater. These models have been modified

for down-gradient calculation of concentrations under uncertainty and have been included in the workstation Advisory System under the acronyms EPAGW (previous section) and EPASF. EPASF addresses the contamination scenarios concerned with impacts in and through surface waters. These are:

Scenario 2A: Violation of an environmental standard in surface water contaminated by leachate. This scenario involves failure of the waste container, followed by transport in groundwater and mixing with uncontaminated stream water.

Scenario 2B: Exposure of humans through drinking water coming from surface water contaminated by leachate. This continues the previous scenario with downstream transport, intake by water treatment plant, and exposure of humans to the contaminant via drinking water.

Scenario 3: Exposure of humans through consumption of fish from surface waters contaminated by leachate carried through groundwater. This proceeds as in Scenario 2A, followed by uptake of contaminant by fish (bioconcentration and/or biomagnification), and human exposure via fish consumption.

All three of these scenarios require calculation of diluted instream concentrations. This may then be equated to standards of human exposure through drinking water and human exposure through consumption of fish, by appropriate assumptions regarding daily water intake and daily average fish consumption. For instance, the pathway analysis through fish consumption is based on an average consumption rate of 6.5 grams of fish per day.

To derive an approximate solution we first assume that the average concentration at the ground water outlet to the surface water, C_g, can be related linearly to the leachate concentration, C_L, as:

$$C_g = z_g C_L$$

where z_g is a groundwater attenuation factor.

It is assumed that the saturated zone transport has reached steady-state. The contaminant mass flux leaching from the site into the groundwater system, m_L, is given by:

$$m_L = Q_L C_L$$

where Q_L is the volumetric rate of leaching from the site, and C_L is the leachate concentration. Solute transport in groundwater from the site to the stream results in

a plume that intercepts the stream over an area A_g with an average concentration C_g. C_g corresponds to the average of the actual point concentration, which is assumed to be a Gaussian distribution over the effective flow area. If the groundwater steady-state seepage velocity is represented by V_g, the contaminant mass flux from the groundwater system into the surface water system, m_g, is given by:

$$m_g = V_g A_g C_g = Q_g C_g$$

where Q_g is the contaminated ground water discharge rate.

At steady state, m_g is related to m_L by:

$$m_g = f_H m_L$$

where f_H is the fraction of the contaminant mass not transformed by hydrolysis or initial speciation in the groundwater (as, at steady state, lateral dispersion of the plume does not affect the total mass loading to the stream).

Combining these equations gives an expression for the concentration dilution factor due to transport in groundwater:

$$Q_L = \frac{f_H Q_L}{Q_g} = z_g$$

The parameters Q_L and f_H are estimated in the simplest case from:

$$Q_L = \frac{P(1 - f_R) A_w}{(86400)(365.25)}$$

and

$$f_H = \exp(-K_g \tau_g)$$

where:

Q_L	=	rate of percolation through the land disposal unit, m^3/sec.
P	=	average annual precipitation rate, m/year.
f_H	=	runoff fraction.
A_w	=	surface area of the waste site, m^2.
K_g	=	total effective decay constant in groundwater, 1/yrs.
τ_g	=	time taken by the contaminant to travel from the land disposal unit to the stream entry point, years.

The factor K_g is estimated exactly as in the model EPAGW. Similarly, the travel time of the constituents in groundwater is given, in the one-dimensional case without dispersion, by:

$$\tau_g = \frac{X_g}{V_g f_{Dg}}$$

where:

X_g	=	distance from site to stream, *m*.
V_g	=	groundwater seepage velocity, *m* / yr.
f_{Dg}	=	fraction of compound that is dissolved, calculated as in the model EPAGW.

When the contaminated ground water enters the stream it mixes with surface water supplied by the upstream watershed. Assuming that the downstream end of the plume entry is given by $x=0$, and that lateral concentration gradients disappear due to mixing, the laterally averaged concentration, C_x increases with x reaching a maximum near the downstream end of the impacting plume ($x=0$).

From mass balance considerations, at $x=0$,

$$C_s = \frac{Q_g}{Q_s^B} C_g = z_s C_g$$

where Q^B_s is the stream base flow at $x=0$, given by:

$$Q_s^B = \frac{P(1-f_R) A_s}{(86400)(365.25)}$$

where A_s is the surface area of the upstream watershed and it is assumed that the average annual precipitation rate, P, and the average runoff coefficient, f_R, are the same for the waste site and the entire watershed. Combining equations then yields the laterally averaged concentration at the downstream edge of the groundwater plume, C_s, as:

$$C_s = \frac{f_H A_w}{A_s} C_L$$

The steady-state laterally averaged value of concentration downstream may then be approximated through an attenuation factor, $z_T = \Theta^{-\beta}$, where $\beta = Kx/U$, K = decay rate constant, sec^{-1}, and U = mean downstream velocity, *m*/sec. In-stream decay processes include sorption, hydrolysis and volatilization. Hydrolysis is calculated dependent on pH and organic carbon fraction of the suspended sediment, in a manner similar to that employed for hydrolysis in EPAGW.

As programmed, the model provides considerable flexibility through the determination of f_H, the mass loading factor, and τ_g, the time taken by the contaminant to travel from the land disposal unit to the stream entry point. The situation described above demonstrates the one-dimensional flow case without dispersion. Options are also included to derive f_H and τ_g with the inclusion of dispersion, using a one-dimensional advection-dispersion solution, and by use of a three-dimensional transport equation. For the latter case, the groundwater transport equation used in determination of f_H is the same as is documented for the model EPAGW.

9. LTIRD, Radial Flow Disposal Systems

The advection-dispersion equation for plane radial flow (Reference 43) may be written as:

$$\frac{1}{r}\frac{\partial}{\partial r}\left[Dr\frac{\partial C}{\partial r}\right] - V\frac{\partial C}{\partial r} = \frac{\partial C}{\partial t}$$

For steady plane radial flow (but transient mass transport), replacing the dispersion coefficient D by $\alpha_L V$, the following expression is obtained (Reference 16):

$$\alpha_L V\frac{\partial^2 C}{\partial r^2} - V\frac{\partial C}{\partial r} = \frac{\partial C}{\partial t}$$

Consider a confined aquifer with thickness b being recharged through a fully penetrating well at a constant rate Q. If the concentration of a chemical in the recharge fluid is C_0 (and the concentration of that chemical in the aquifer water was originally zero), the equation above may be rewritten as:

$$\frac{1}{r_D}\frac{\partial^2 C_D}{\partial R_D^2} - \frac{1}{r_D}\frac{\partial C_D}{\partial r_D} = \frac{\partial C_D}{\partial t_D}$$

where:

$$r_D = \frac{r}{\alpha_l}$$

$$t_D = \frac{Qt}{2\pi b n \alpha_L^2}$$

$$C_D = \frac{C}{C_0}$$

Initial and boundary conditions for this problem are:

$$C_D\,(r_D\,,\,t_D\,) = 0, \quad t_D=0$$

$$C_D\,(r_{D_w},\,t_D\,) = 1$$

$$\lim_{r_D \to \infty} C_D\,(r_D,\,t_D\,) = 0$$

where r_{Dw} is the dimensionless well (source) diameter. The solution in the Laplace transform domain, in terms of Airy functions, is:

$$L_D = \frac{1}{s}\,\exp\left[\frac{r_D - R_D w}{2}\right]\left[\frac{Ai\,(Y\,)}{Ai\,(Y_O\,)}\right]$$

where:

L_D	=	Laplace transform of dimensionless concentration.
s	=	Laplace transform parameter.
Y	=	$s^{-2/3}\,(sr_D + \frac{1}{4})$
Y_0	=	$s^{-2/3}\,(sr_{Dw} + \frac{1}{4})$

The general form of the Airy function can be found in Abramowitz and Stegun (Reference 46). An asymptotic expansion yields:

$$Ai\,(z) \approx \frac{1}{2}\,\sqrt{\pi}\;z^{-1/4}\;e^{-\xi}\sum_{k=0}^{\infty}\;(-1)^k\,c_k\,\xi^{-k}$$

$$for \quad |z| < 1$$

where:

$$c_k = \frac{(2k+1)\,(2k+3)\,\ldots(6k-1)}{216^k\,k!}$$

$$c_0 = 1$$

$$\xi = \frac{2}{3}\,z^{3/2}$$

The computer code LTIRD calculates the dimensionless concentration of a solute injected into an aquifer. It has been adapted for single rotary distributors in the workstation Advisory System, but should not be used for multiple distributors.

10. RESSQ, Semi-analytical Model Based On Complex Velocity Potential

Semi-analytical methods are more powerful than analytic methods in terms of representation of the flow regime, and simpler than most of the complete numerical techniques. These methods apply a well-known concept of fluid mechanics: the complex velocity potential. A major limitation is that they apply only to steady-state two-dimensional fluid flow through homogeneous media. The computer program RESSQ calculates two-dimensional contaminant transport by advection and adsorption (no dispersion or diffusion) in a homogeneous, isotropic confined aquifer of uniform thickness when regional flow, sources and sinks create a steady-state flow field (Reference 16).

The velocity potential is generally defined as:

$$\phi = Kh + c$$

Therefore, a component of the specific discharge or Darcy velocity vector in any arbitrary direction x is:

$$q_x = -\frac{\partial \phi}{\partial x} = -K\frac{\partial h}{\partial x}$$

The stream function can be obtained with a known velocity potential by using the Cauchy-Riemann equations:

$$\frac{\partial \phi}{\partial x} = \frac{\partial \psi}{\partial y}$$

$$\frac{\partial \phi}{\partial y} = -\frac{\partial \psi}{\partial x}$$

Both the stream function and velocity potential are harmonic functions in that they satisfy the Laplace equation: therefore, their application is restricted to steady-state planar flow fields. The complex velocity potential of a uniform flow with Darcy velocity U, in a direction making an angle α with the positive x axis, is:

$$W = -UZe^{-i\alpha} + c$$

Substituting for complex numbers Z and $e^{-i\alpha}$, the velocity potential and the stream function for such a flow system are obtained:

$$W = \phi + i\psi = -U(x + iy)(\cos\alpha - i \sin\alpha) + c$$

$$\phi = -U(x \cos\alpha + y \sin\alpha) = constant$$

$$\psi = U(x \sin\alpha - y \cos\alpha) = constant$$

The latter two equations represent equipotentials and streamlines, respectively. Components of specific discharge are:

$$q_x = -\frac{\partial\phi}{\partial x} = U\cos\alpha$$

$$q_y = -\frac{\partial\phi}{\partial y} = U\sin\alpha$$

The complex velocity potential of a source with strength m located at the point Z_0 is:

$$W = m \ln (Z - Z_0) + c$$

If the source represents a well which is being recharged at rate Q into an aquifer of thickness b, then the strength m of the source is simply:

$$m = -\frac{Q}{2\pi b}$$

Substituting for complex numbers Z and Z_0, the velocity potential and stream function are:

$$W = \frac{-Q}{2\pi b} \ln \sqrt{(x - x_0)^2 + (y - y_0)^2} - i \frac{Q}{2\pi b} \tan^{-1}\left[\frac{y - y_0}{x - x_0}\right] + c$$

$$\phi = \frac{-Q}{4\pi b} \ln [(x - x_0)^2 + (y - y_0)^2] + c_1$$

$$\psi = \frac{-Q}{2\pi b} \tan^{-1}\left[\frac{(y - y_0)}{(x - x_0)}\right] + c_2$$

where x_0 and y_0 are the coordinates of the source and x and y are the coordinates of

a point where the velocity potential and stream function are calculated. Components of specific discharge based on the above definitions are:

$$q_x = -\frac{\partial \phi}{\partial x} = \frac{Q}{2\pi b}\,\frac{(x - x_0)}{(x - x_0)^2 + (y - y_0)^2}$$

$$q_y = -\frac{\partial \phi}{\partial y} = \frac{Q}{2\pi b}\,\frac{(y - y_0)}{(x - x_0)^2 + (y - y_0)^2}$$

The complex velocity potential for a positive doublet is:

$$W = \frac{\Omega \bar{Z}}{|Z|^2} + C$$

where

$\bar{Z}$ = *conjugate of complex number Z, and*
$|Z|$ = *modulus of complex number Z.*

Substituting for these two values, the velocity potential and stream function for a positive doublet located at the origin are:

$$W = \phi + i\psi = \frac{\Omega (x - iy)}{x^2 + y^2}$$

$$\phi = \frac{\Omega x}{x^2 + y^2} = \textit{constant}$$

$$\psi = \frac{-\Omega y}{x^2 + y^2} = \textit{constant}$$

The latter two equations can be rearranged to give:

$$\left[x - \frac{\Omega}{2c}\right]^2 + y^2 = \left[\frac{\Omega}{2c}\right]^2$$

$$x^2 + \left[y + \frac{\Omega}{2c}\right]^2 = \left[\frac{\Omega}{2c}\right]^2$$

The first equation represents equipotentials and describes circles with centers along the *x* axis. Similarly, the second equation represents a group of circles with centers

on the *y* axis and tangent to the *x* axis. These circles are the streamlines for such a doublet.

Since the Laplace equation is a linear partial differential equation, the principle of superposition applies: as many flow components as needed can be superimposed to obtain the expression for the complex velocity potential of an entire system. For example, one or several point sources of contaminant recharge, together with some groundwater discharge wells, can be combined with a uniform regional groundwater flow regime. The overall complex velocity potential may be written as:

$$W = -UZ^{ia} + \sum_{j=1}^{N} \frac{Q}{2\pi b} \ln (Z - Z_j) - \sum_{k=1}^{M} \frac{Q_k}{2\pi b} \ln (Z - Z_k) + c$$

where:

W	=	overall complex velocity potential of the system.
U	=	Darcy velocity of uniform regional flow.
a	=	angle between the direction of regional flow and the positive x axis.
b	=	aquifer thickness.
Q_j	=	rate of discharge from well j.
Q_k	=	rate of discharge from well k.

The velocity potential of the above system, the real part of W, is (Reference 16):

$$\phi = -U(x \cos\alpha + y \sin\alpha) + \sum_{j=1}^{N} \frac{Q}{4\pi b} \ln [(x-x_j)^2 + (y-y_j)^2]$$

$$- \sum_{k=1}^{M} \frac{Q_k}{4\pi b} \ln [(x-x_k) + (y-y_k)^2] + c_1$$

and the expression for the stream function, the imaginary part of W, becomes:

$$\psi = U(x \sin\alpha - y \cos\alpha) + \sum_{j=1}^{N} \frac{Q}{2\pi b} \tan^{-1} \left[\frac{y-y_j}{x-x_j}\right]$$

$$- \sum_{k=1}^{M} \frac{Q_k}{2\pi b} \tan^{-1} \left[\frac{y-y_k}{x-x_k}\right] + c_2$$

At any given point with coordinate (x,y), components of the specific discharge for the overall system may be written as:

$$q_x = -\frac{\partial \phi}{\partial x} = U\cos\alpha - \sum_{j=1}^{N} \frac{Q}{2\pi b} \frac{(x-x_j)}{(x-x_j)^2 + (y-y_j)^2} + \sum_{k=1}^{M} \frac{Q_k}{2\pi b} \frac{(x-x_k)}{(x-x_k)^2 + (y-y_k)^2}$$

$$q_y = -\frac{\partial \phi}{\partial y} = U\sin\alpha - \sum_{j=1}^{N} \frac{Q}{2\pi b} \frac{(y-y_j)}{(x-x_j)^2 + (y-y_j)^2} + \sum_{k=1}^{M} \frac{Q_k}{2\pi b} \frac{(y-y_k)}{(x-x_k)^2 + (y-y_k)^2}$$

Components of the average pore water velocity for an individual fluid particle moving through the overall flow system are (by introducing a retardation factor, R):

$$v_{cx} = \frac{q_x}{nR}$$

$$v_{cy} = \frac{q_y}{nR}$$

The path line travelled by a contaminant particle can be divided into increments dl, traversed in time intervals dt. The projections of dl on the x and y axes are given by dx and dy, respectively:

$$dx = v_{cx}\,dt = \frac{q_x\,dt}{nR}$$

$$dy = v_{cy}\,dt = \frac{q_y\,dt}{nR}$$

$$dl = \sqrt{(dx^2 + dy^2)} = \sqrt{(q_x^2 + q_y^2)}\ \frac{dt}{nR}$$

Numerical integration of the equation for dl yields travel time between any two points of a given streamline. If a contaminant particle is at a point (x_j, y_j) at time t, its new position at time $t + dt$ on the same streamline can be calculated by using:

$$x_{j+1} = x_j + \Delta x = x_j + \frac{q_x \Delta t}{nR}$$

$$y_{j+1} = y_j + \Delta y = y_j + \frac{q_y \Delta t}{nR}$$

According to Javandel *et al.* (Reference 16), the combination of a uniform flow in the positive x direction with a positive doublet and a point source (both centered at the origin) represents outflow from a completely penetrating cylindrical pond in the presence of a uniform flow in the positive x direction. The complex velocity potential, then, is:

$$W = -UZ + \frac{\Omega \bar{Z}}{|Z|^2} - \frac{Q_p}{2\pi b} \ln Z + c$$

and the velocity potential and stream function are:

$$\phi = -Ux + \frac{\Omega x}{x^2 + y^2} - \frac{Q_p}{4\pi b} \ln (x^2 + y^2) + c_1$$

$$\psi = -Uy + \frac{\Omega y}{x^2 + y^2} - \frac{Q_p}{2\pi b} \tan^{-1}\left(\frac{y}{x}\right) + c_2$$

where:

U	=	Darcy velocity of uniform flow in the positive x direction.
Q_p	=	rate of outflow from the pond.
b	=	thickness of the aquifer.
Ω	=	constant of the doublet.

The value of the constants in the velocity potential equation can be determined such that the velocity potential satisfies the appropriate boundary conditions. Holding ϕ constant and equal to H_0 at $r = r_0$,

$$\phi = H_0 - Ux + \frac{Ur_0^2 x}{x^2 + y^2} - \frac{Q_p}{4\pi b} \ln \left[\frac{x^2 + y^2}{r_0^2}\right]$$

Incorporating the velocity potential of sources and sinks, the result is:

$$\phi = H_0 - Ux + \frac{Ur_0^2 x}{x^2 + y^2} - \frac{Q_p}{4\pi b} \ln \left[\frac{x^2 + y^2}{r_0^2}\right]$$
$$+ \sum_{j=1}^{M} \frac{Q_j}{4\pi b} \ln \left[\frac{(x-x_j)^2 + (y-y_j)^2}{x_j^2 + y_j^2}\right]$$
$$- \sum_{k=1}^{M} \frac{Q_k}{4\pi b} \ln \left[\frac{(x-x_k)^2 + (y-y_k)^2}{x_k^2 + y_k^2}\right]$$

where Q_j and Q_k are the rates of discharge and recharge of sinks and sources, respectively. Components of the average pore water velocity at any point (x,y) within the overall flow regime where the velocity potential is defined may be written as:

$$v_x = -\frac{1}{n}\frac{\partial \phi}{\partial x} = \frac{U}{n} + \frac{Ur_0^2}{n}\left[\frac{x^2 - y^2}{(x^2 + y^2)^2}\right] + \frac{Q_p}{2\pi nb}\frac{x}{x^2 + y^2}$$
$$- \sum_{j=1}^{N} \frac{Q_j}{2\pi nb}\frac{(x-x_j)}{(x-x_j)^2 + (y-y_j)^2} + \sum_{k=1}^{M} \frac{Q_k}{2\pi nb}\frac{(x-x_k)}{(x-x_k)^2 + (y-y_k)^2}$$

and

$$v_y = -\frac{1}{n}\frac{\partial \phi}{\partial y} = \frac{Ur_0^2}{n}\left[\frac{2xy}{(x^2 + y^2)^2}\right] + \frac{Q_p}{2\pi nb}\frac{y}{x^2 + y^2}$$
$$- \sum_{j=1}^{N} \frac{Q_j}{2\pi nb}\frac{(y-y_j)}{(x-x_j)^2 + (y-y_j)^2} + \sum_{k=1}^{M} \frac{Q_k}{2\pi nb}\frac{(y-y_k)}{(x-x_k)^2 + (y-y_k)^2}$$

11. MOC, Method of Characteristics Two-Dimensional Solute Transport Model

This model can be applied to a wide variety of one- and two-dimensional problems involving steady-state or transient flow. It computes changes in concentration due to the following processes (References 21, 22 and 23) :

a. convective transport by which dissolved chemicals move with the flowing groundwater;

b. hydrodynamic dispersion, by which molecular and ionic diffusion

and small-scale variations in the velocity of flow through the porous media cause the path of dissolved molecules or ions to spread from the average direction of groundwater flow;

c. fluid sources, causing mixing or dilution;

d. reactions, by which the concentration of chemical is modified by its interaction with other species present in the groundwater solution or the solid aquifer materials.

The model assumes that the gradients of fluid density, viscosity and temperature do not affect the velocity distribution. The solute can be reactive or conservative, and the aquifer can be heterogeneous and/or anisotropic. The computer program first solves the governing equation that describes the transient two-dimensional areal flow of a homogeneous compressible fluid through a nonhomogeneous anisotropic aquifer:

$$\frac{\partial}{\partial x_i}\left(T_{ij}\,\frac{\partial h}{\partial x_j}\right) = S\,\frac{\partial h}{\partial t} + W$$

where

T_{ij} = transmissivity tensor (L^2/T) = $K_{ij}b$
K_{ij} = hydraulic conductivity tensor (L/T)
S = storage coefficient
W = source or sink term
x_i = cartesian coordinates (L)
h = hydraulic head (L)
b = aquifer thickness (L).

The source or sink term, W, is the volume flux per unit area. When only the following terms are considered: (a) direct withdrawal or pumpage (well pumpage, evapotranspiration or well injection); (b) steady leakage into or out of the aquifer through a confining layer, then the term W may be expressed as

$$W(x, y, t) = Q(x, y, t) - \frac{K_z}{m}\,(H_s - h)$$

where

Q = rate of withdrawal (positive sign) or recharge (negative sign), (L/T);
K_z = vertical hydraulic conductivity of the confining layer, (L/T); m = thickness of the confining layer, (L);

H_s = hydraulic head in the source, (L).

Darcy's Law provides a basis to calculate the average seepage velocity of groundwater:

$$V_i = -\frac{K_{ij}}{\epsilon} \frac{\partial h}{\partial x_j}$$

where

V_i = seepage velocity in the direction of x_i (L/T);
ϵ = effective porosity of the aquifer.

The mass transport equation is:

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x_i}\left(D_{ij} \frac{\partial C}{\partial x_j}\right) - \frac{\partial}{\partial x_i}(CV_i) - \frac{C_0 W}{\epsilon b} + \sum_{k=1}^{m} R_k$$

where

C = concentration of solute (M/L^3);
D_{ij} = coefficient of dispersion (L^2/T);
C_o = solute concentration in source or sink fluid (M/L^3);
R_k = rate of addition or removal of solute by physical or chemical reactions (M/L^3T);
b = saturated thickness of the aquifer (L).

The first term on the right-hand side of the transport equation describes the hydrodynamic dispersion, the second term represents the convective transport, and the third and fourth term describe, respectively, fluid sources or sinks and changes in concentration due to chemical or physical reactions occurring in the groundwater solution. The first step in solving this equation is to estimate the value of D_{ij}. According to Scheidegger (Reference 47), the dispersion coefficient can be computed as a function of the velocity of groundwater flow and the nature of the aquifer. Assuming that the molecular diffusion is negligible,

$$D_{ij} = \alpha_{ijmn} \frac{V_m V_n}{|V|}$$

and

$$|V| = \sqrt{V_x^2 + V_y^2}$$

where

α_{ijmn} = dispersivity of the aquifer (L);
V_m, V_n = components of velocity in the m and n directions, respectively (L/T).

For an isotropic medium, the dispersivity tensor may be defined in terms of the longitudinal and transverse dispersivities of the aquifer (α_L and α_T, respectively). The components of the dispersion coefficient may be described as:

$$D_{xx} = \alpha_L \frac{V_x^2}{|V|} + \alpha_T \frac{V_y^2}{|V|}$$

$$D_{yy} = \alpha_L \frac{V_y^2}{|V|} + \alpha_T \frac{V_x^2}{|V|}$$

$$D_{xy} = D_{yx} = (D_L - D_T) \frac{V_x V_y}{|V|^2}$$

where $D_L = \alpha_L \mid V \mid$ and $D_T = \alpha_T \mid V \mid$ are the longitudinal and transverse dispersion coefficients.

The sequence of steps involved in solving these equations is to determine the velocity distribution from the flow equation and Darcy's Law. Next, given the values of α_L and α_T, Darcy's Law is solved subject to certain boundary and initial conditions. Flow and mass transport equations are treated as uncoupled equations in that concentration changes do not affect the flow field; this applies where density differences are negligible, which is the case in most contaminant problems, and one of the assumptions in the MOC model. There are two situations where solutions to the previous equations may be applied: (1) to assess the impact of proposed subsurface waste disposal sites that have not yet been contaminated; (2) to assess the impact of already contaminated sites, predict plume migration and recommend remedial actions.

Numerical Solution

Exact analytical solutions to the partial differential equations of flow and solute mass transport cannot be obtained directly due to vari[illegible]roperties of aquifers and complex boundary conditions. The solutions must be [illegible]oximated by a numerical scheme. The basic method is to break up continuous space into cells, approximate the governing partial differential equations by differences between the values of the

parameters over the network and then compute the discrete parcel. MOC utilizes a rectangular, uniformly spaced, block-centered, finite-difference grid—in which nodes are defined at the centers of the rectangular cells.

The numerical solution technique first solves the equation describing the transient two-dimensional flow of a homogeneous fluid through a nonhomogeneous anisotropic aquifer with the following implicit finite-difference approximation:

$$T_{xx[i-1/2,j]} \frac{h_{i-1,j,k}-h_{i,j,k}}{(\Delta x)^2} + T_{xx[i+1/2,j]} \frac{h_{i+1,j,k}-h_{i,j,k}}{(\Delta x)^2}$$

$$+ T_{yy[i,j-1/2]} \frac{h_{i,j-1,k}-h_{i,j,k}}{(\Delta y)^2} + T_{yy[i,j+1/2]} \frac{h_{i,j+1,k}-h_{i,j,k}}{(\Delta y)^2}$$

$$= S \frac{h_{i,j,k}-h_{i,j,k-1}}{(\Delta t)} + \frac{q_{w(i,j)}}{\Delta x \Delta y} \frac{K_z}{m} (H_{s(i,j)}-h_{i,j,k})$$

where i,j,k = indices in the x,y, and t dimensions, respectively;

Δx, Δy, Δt = increments in the x,y and time dimensions, respectively;

q_w = volumetric rate of withdrawal or recharge at the (i,j) node (L^3/T).

This equation is solved numerically for each node in the grid using an iterative alternating-direction-implicit (ADI) procedure (References 24, 48, and 49). After the head distribution is computed, the velocity of the groundwater flow is computed for each node using an explicit finite difference form of Darcy's equation:

$$V_{x(i,j)} = -\frac{K_{(i,j,k)}}{\epsilon} \frac{h_{i-1,j,k} - h_{i+1,j,k}}{2\Delta x}$$

Next, the solute transport equation is solved. This equation describes the two-dimensional areal transport and dispersion of a given reactive dissolved chemical species in flowing groundwater. This equation is solved using the method of characteristics, through a three step procedure. If saturated thickness is considered as a variable and the convective transport term is expanded, the mass transport equation may be rewritten as

$$\frac{\partial C}{\partial t} = \frac{1}{b} \frac{\partial}{\partial x_i} \left[b D_{ij} \frac{\partial C}{\partial x_j} \right] - V_x \frac{\partial C}{\partial x_i} - V_y \frac{C}{\partial x_j} + \frac{W(C-C')}{\epsilon\, b} + \sum_{k=1}^{m} R_k$$

which is in the form solved by the computer program.

Changes with time in properties of the fluid (e.g., concentration) may be

described either for fixed points within a stationary coordinate system as succesive particles pass the reference points, or for reference fluid particles as they move along their respective paths past fixed points in space. The derivative $\partial C/\partial t$ is the rate of change of concentration as observed from a fixed point, whereas dC/dt is the rate of change as observed when moving with the fluid particle (material derivative).

- **Particle tracking.** This first step solved for the change in concentration over distance. It consists of placing a number of traceable particles in each cell of the finite-difference grid, to form a set of points that are distributed in a geometrically uniform pattern throughout the area of interest. The location of each particle is specified by its *x* and *y* coordinates. The initial concentration assigned to each point is the initial concentration at the node of the cell containing the particle. For each time step every point is moved a distance proportional to the length of the time increment and the velocity at the location of the point. The new position of the particle is then computed and, after all points have been moved, the concentration at each node is temporarily assigned the average of the concentrations of all points located within the area of that cell.

A two-step explicit finite-difference approximation is now used to calculate the new nodal concentrations at the end of the time period. The changes in concentration caused by hydrodynamic dispersion, fluid sources, divergence in velocity, changes in saturated thickness, adsorption or chemical reaction are calculated using an explicit finite-difference approximation. This change in concentration can be considered as the sum of two separate terms:

$$\Delta C_{i,j,k} = (\Delta C_{i,j,k})_I + (\Delta C_{i,j,k})_{II}$$

where the subscript *I* represents the change in concentration caused by hydrodynamic dispersion, and the subscript *II* is the change caused by an external fluid source, changes in saturated thickness, adsorption or chemical reaction:

$$(\Delta C_{i,j,k})_I = \frac{\Delta t}{b}\left[\frac{\partial}{\partial x_i}\left(b D_{ij}\ \frac{\partial C}{\partial x_j}\right)\right]$$

$$(\Delta C_{i,j,k})_{II} = \frac{\Delta W_{i,j,k}}{\epsilon\ b_{i,j,k}}\left[C_{i,j,k-1} - C_{i,j,k}\right]$$

Later modifications (References 22 and 23) include first-order radioactive decay (λ), and retardation factors (R_f) for linear sorption, non-linear sorption and ion exchange.

$$\textit{Decay:}\quad \lambda = \frac{\ln 2}{t_{1/2}}$$

where $t_{1/2}$ is the half-life of the solute, (T). For example,

$$\textit{Linear Sorption} : \quad R_f = 1 + \frac{\rho_b K_d}{\epsilon}$$

$$\textit{Nonlinear Sorption} : \quad R_f(C) = 1 + \frac{\rho_b}{\epsilon} \frac{d\bar{C}}{dC}$$

The decay is applied directly to the tracer particles (rather than at the nodes of the finite difference grid):

$$C_p^k = C_p^{k-1} \exp(-\lambda \Delta t)$$

where

c_p = solute concentration of the tracer particle, and
k = time dimension index.

The exponential decay formulation has no numerical stability restrictions, but some numerical accuracy is lost if the half-life is much smaller than the time step for solving the transport equation.

- **Stability criteria.** The explicit numerical solution of the solute-transport equation has some stability criteria associated with it, which may require that the time step used to solve the flow equation be subdivided into a number of smaller time increments to accurately solve the solute-transport equation. The stability criteria may be stated as follows:

$$\Delta t \leq \left(\begin{matrix} \text{Min} \\ \text{over} \\ \text{grid} \end{matrix} \right) \left[\frac{0.5}{\frac{D_{xx}}{(\Delta x)^2} + \frac{D_{yy}}{(\Delta y)^2}} \right]$$

$$\Delta t \leq \left(\begin{matrix} \text{Min} \\ \text{over} \\ \text{grid} \end{matrix} \right) \left[\frac{\epsilon \, b_{i,j,k}}{W_{i,j,k}} \right]$$

$$\Delta t \leq \frac{\gamma \, \Delta x}{(V_x)_{max}}$$

$$\Delta t \leq \frac{\gamma \Delta y}{(V_y)_{max}}$$

where γ is the fraction of the grid dimensions that particles are allowed to move at each time step ($0 \leq \gamma \leq 1$).

If the time step used to solve the flow equation exceeds the smallest of the time limits determined by the above equations, then the time step will be subdivided into the appropriate number of smaller time increments required for solving the solute-transport equation.

- **Boundary and initial conditions.** Several different types of boundary conditions can be incorporated into the solute transport model. Two general types have been used in this model: constant flux and constant-head conditions. A constant head boundary can be used to represent aquifer underflow, well withdrawals or well injection. A finite flux is defined by specifying the flux rate as a well discharge or injection rate for the appropriate nodes. A no-flow boundary is a special case of a constant flux boundary. The numerical procedure requires that the area of interest be surrounded by a no-flow boundary. No-flow boundaries can also be located elsewhere in the grid to represent natural barriers to groundwater flow. No-flow boundaries are designated by setting to zero the transmissivity at appropriate nodes.

A constant-head boundary represents parts of the aquifer such as recharge boundaries or areas beyond the influence of hydraulic stress. Constant-head boundaries are represented by adjusting the leakage term at appropriate nodes. If a constant-flux or constant-head represents a fluid source, then the chemical concentration in the source fluid must also be specified. The initial conditions can be determined from field data and from previous simulations. The head and concentration in the aquifer at the start of the simulation must be specified, because solute transport depends directly upon hydraulic and concentration gradients.

Monte Carlo Simulation Option

The MOC model as described in the preceding sections involves a large degree of uncertainty originated by the combination of model error, natural and parameter uncertainties. As an alternative to the deterministic approach in which detailed data are required for the simulation, the Monte Carlo technique enables a prediction which incorporates the uncertainty associated to the inputs and parameters of the model. This is achieved by a random generation of the most sensitive inputs to the model, followed by a large number of computations to yield a well defined distribution of outputs.

12. HELP, Hydrologic Evaluation Of Landfill Performance

The Hydrologic Evaluation of Landfill Performance (HELP) model was developed to facilitate rapid, economical estimation of the amounts of surface runoff, subsurface drainage, and leachate that may be expected to result from the operation of a wide variety of possible landfill designs (Reference 51). These phenomena arise from the interaction of a large number of complex hydrologic processes, including precipitation, surface storage, runoff, infiltration, percolation, evapotranspiration, soil moisture storage and lateral drainage. HELP takes what is essentially a water-balance approach to the problem, within a quasi-two dimensional process. The model uses climatologic, soil, and design data to produce estimates of water movement across, into, through, and out of landfills. To accomplish this, daily precipitation is partitioned into surface storage (snow), runoff, infiltration, surface evaporation, evapotranspiration, percolation, stored soil moisture, and subsurface lateral drainage to maintain a water budget. Calculations may be performed for up to nine layers of a landfill design. These layers may include a vegetative layer, other types of vertical percolation layers, lateral drainage layers, barrier soil layers and waste layers.

Surface Runoff. Surface runoff is computed by the SCS curve number technique (Reference 51). This method was chosen by the authors because it is well established, easy to use, and the required input data is generally available. Generally, the curve number for a watershed is determined for average moisture conditions in the SCS method (CN_{II}). The curve number for the lowest antecedent moisture conditions, CN_I, is related to CN_{II} by a polynomial developed for the CREAMS model (Reference 52):

$$CN_I = -16.91 + 1.348\ CN_{II} - 0.01379\ CN_{II}^{\ 2} + 0.0001177\ CN_{II}^{\ 3}$$

The maximum retention factor for a soil, S_{mx} is then determined from:

$$S_{mx} = \frac{1000}{CN_I} - 10$$

From this information we can calculate the daily depth weighted retention factor, S_i, and the daily runoff, Q_i, using the method documented by Knisel (Reference 52). The soil profile of the vegetative or evaporative depth was divided into seven segments. The thickness of the top segment was set equal to 1/36 of the thickness of this depth, while the thickness of the second segment was 5/36 of this depth. Each of the remaining 5 segments was defined as 1/6 of the thickness of the vegetative or evaporative depth. We may then state:

$$S_I = \left\{ 1 - \sum_{j=1}^{7} W_j \left(\frac{SM_j - WP_j}{UL_j - WP_j} \right) \right\}$$

where

SM_j = soil water content of segment j, inches
UL_j = saturated capacity of segment j, inches
WP_j = wilting point of segment j, inches

and

$$W_j = 1.0159 \left\{ \exp\left(-4.16 \frac{D_j - 1}{VD}\right) - \exp\left(-4.16 \frac{D_j}{VD}\right) \right\}$$

where:

D_j = depth to bottom of segment j, inches
VD = vegetative or evaporative depth, inches.

and

$$Q = \frac{(P - 0.2S)^2}{(P + 0.8S)}$$

where:

P = actual rainfall
S = maximum retention including the initial abstraction.

Infiltration. Infiltration is equal to the difference between the daily precipitation, the sum of the change in the surface storage of precipitation (snow), the daily runoff, and the surface evaporation. Thus the net daily infiltration, IN_i, is given by:

$$IN_i = P_i - Q_i - ESS_i$$

where

ESS_i = surface water evaporation on day i, inches.
Q_i = daily runoff, inches.
P_i = net rainfall, given by:

$$p_i = PRE_i - SNO_{i-1} - SNO_i$$

where:

PRE_i = actual precipitation on day i, in inches.
SNO_i = amount of snowwater at end of day i, inches.

Evapotranspiration. The potential evapotranspiration calculation is also adapted from Knisel (Reference 52), and is computed using a modified Penman method developed by Ritchie (Reference 53). The potential evapotranspiration on day i, E_{oi}, is given by:

$$E_{o_i} = \frac{1.28\ A_i H_i}{(A_i + G)\ 25.4}$$

where:

H_i = net solar radiation on day i, langleys.
G = psychrometric constant which equals 0.68
A_i = slope of saturation vapor pressure curve on day i, computed from:

$$A_i = \frac{5304}{T_i^2} \exp\left(\frac{21.255 - 5304}{T_i}\right)$$

where:

T_i = mean temperature in °K on day i.

The daily potential evapotranspiration demand is applied first on water available on the surface. Any demand in excess of the surface water is exerted on the soil column in the forms of soil evaporation and plant transpiration. The potential soil evaporation, ES_{oi}, is given by:

$$ES_{o_i} = E_{o_i}\ e^{-0.4\ LAI_i}$$

where LAI_i is the leaf area index on day i, or the winter cover factor in non-growing seasons. Soil evaporation proceeds at this rate when evaporation is not limited by transmission of water to the surface. Again following Knisel (Reference 52), this limit is given by:

$$U = \frac{9\ (a_s - 3)^{0.42}}{25.4}$$

where a_s = soil transmissivity parameter for evaporation, $(mm/day)^{0.5}$.

After reaching this limit, soil evaporation proceeds at a stage-two rate, $ES2_i$, given by:

$$ES2_i = \frac{\sqrt{t_i} - \sqrt{(t_i - 1)}}{25.4}$$

where t_i = days since stage one evaporation ended.

The potential plant transpiration, EP_{oi}, is computed from:

$$EP_{o_i} = \frac{E_{o_i}\ LAI_i}{3}$$

Actual plant transpiration depends on soil moisture and plant transpiration demand, where the plant transpiration demand, EPD_i, is equal to the potential plant transpiration except when limited by low soil moisture or when the daily total of the surface evaporation, soil evaporation and plant transpiration exceeds the daily potential evapotranspiration. The actual plant transpiration, EP_i is then given by:

$$EP_i = EPD_i \left[1.20 - (4\ EPD_i) + \frac{SM_i - WP}{FC - WP} \right]$$

in which:

SM_i = depth weighted soil moisture on day i,
WP = depth weighted wilting point,
FC = depth weighted field capacity.

Full details of the weighting procedure are given in Schroeder *et al.* (Reference 50).

Soil Moisture Storage. The HELP model uses a daily time interval to evaluate the components of the water balance equation. Soil moisture storage is then given in general terms as:

$$SM_i = SM_{i-1} + \frac{1}{2} (IN_i - PE_i - ET_i + IN_{i-1} - PE_{i-1} - ET_{i-1})$$

where:

SM_i = soil moisture storage at midday i
IN_i = infiltration on day i
PE_i = percolation and drainage from landfill on day i
ET_i = evapotranspiration on day i

In application of the model the vegetative or evaporative zone is divided into seven segments. Soil water is then distributed among these segments and all underlying layers, with the equations connected by vertical drainage terms. The model assumes that barrier layers always remain at saturation. After distributing the water among the layers the model checks to see that the soil moisture storage does not exceed the saturated capacity. Any excess above this amount is added to the soil moisture storage of the layer above, or, if an excess in the topmost segment, added to the surface runoff.

Vertical Flow. The model assumes that the soil profile consists of discrete segments that are homogeneous with respect to the hydraulic conductivity, the total porosity and field capacity. The rate of downward flow is assumed to follow Darcy's law. However, it is further assumed that free outflow occurs from each segment above the barrier soil layer, in which case the rate of flow equals the hydraulic

conductivity, k. This assumption is valid as long as the hydraulic conductivities of the segments above the barrier soil layer are similar, or increase with increasing depths of the segments. The effective hydraulic conductivity, k_v, is a function of the saturated hydraulic conductivity, k_s, and the soil moisture content, defined through:

$$k_v = k_s \left(\frac{SM_l - MDC}{UL - MDC} \right)$$

where *MDC* is the minimum soil water content for drainage to occur.

The routing of moisture from segment to segment is done using a routing procedure computed at the mid-point of the time interval, proceeding sequentially from the top segment to the bottom segment. The model then solves simultaneously for drainage rate and soil moisture. If the moisture content of a segment is greater than its total porosity the excess is backed up into the segment above it.

After convergence is obtained for the segments above a barrier layer, the hydraulic head may be computed on the barrier. Flow through the barrier layer is then also computed using Darcy's Law, as:

$$q = k_s \frac{TH + TS(n+1)}{TS(n+1)}$$

where:

k_s	=	saturated hydraulic conductivity of the barrier layer
TH	=	total head on the barrier layer
$TS(n+1)$	=	thickness of the barrier soil layer.

Lateral Flow. The lateral drainage procedure is based on the Boussinesq equation, which is unsteady and non-linear:

$$f \frac{\partial h}{\partial t} = K \frac{\partial}{\partial x}\left[(h - x\alpha) \frac{\partial h}{\partial x} \right] + R$$

where:

f	=	dimensionless drainable porosity
t	=	time in days
h	=	gravitational head in inches
K	=	effective saturated lateral hydraulic conductivity, inches/day
x	=	lateral position in the direction of drainage
α	=	dimensionless slope
R	=	recharge flux in inches/day perpendicular to the direction of flow

With the selection of a small time step, the steady state assumption is made, $\partial h/\partial t = 0$. The equation is then linearized following the form given by Skaggs (Reference 54), but incorporating an additional correction factor developed by Schroeder *et al.* (Reference 50). This yields the approximate relationship for lateral drainage, *QLAT*, as:

$$QLAT = \frac{2\,(0.510 + 0.00205\,\alpha L)\;Ky[y\,(y/L)^{0.16} + \alpha L]}{L^2}$$

where:

L	=	lateral distance from the crest to the drain, inches
y	=	average thickness of water profile above barrier soil layer between $x=0$ and $x=L$, inches.

The vertical and lateral flow routines are then linked under two assumptions: (1) steady-state conditions hold such that change in head is not a function of time, and (2) the drainage rate estimated at the mid-point of the time interval is effective throughout the time interval. These assumptions are valid only if the computational time interval is sufficiently small so that there is little change in head. The model is set to use a time step appropriate for most common conditions. The authors contend that four equal time steps per day yields acceptable accuracy for heads less than 30 inches. Finally, the model must perform a convergence to ensure that the drainage rate from the bottom of the profile is equal to the sum of lateral flow and vertical percolation. The results are converged to the 5% level by an iterative scheme commencing with an *a priori* estimate of drainage rate from the bottom profile' segment. This estimate is updated until convergence within the 5% level is obtained.

SECTION III

APPLICATIONS

By searching the Air Force IRPIMS data base, it was determined that Hill AFB (located about 25 miles north of Salt Lake City and 5 miles south of Ogden, Utah) had several sites that are good candidates for mathematical modeling. This was confirmed after a 2-day visit to Hill AFB (June 25-26, 1990) by the first writer, as an Air Force-UES Summer Faculty Fellow at Brooks AFB, Texas. Hydrogeologic and contaminant transport data were requested for these sites: a limited amount of data was obtained for Operable Unit 3 (OU3) at Hill AFB (References 55 and 56).

A. APPLICATION OF ODAST

The one-dimensional analytical model ODAST was applied by James M. Montgomery (Reference 56) to illustrate the relationship between OU3 sources and contaminant migration. The model assumes that the aquifer is homogeneous and isotropic with steady-state uniform groundwater flow at constant velocity. It calculates the contaminant concentration at any time, at any longitudinal distance from the source — based on the length of time the contaminant was injected into the groundwater, and it adjusts the concentration for dispersion and retardation. The resulting concentration profile is presented in Figure 6.

B. APPLICATION OF MOC AND REMEDIATION OPTIMIZATION

The two-dimensional flow and transport model developed by Konikow and Bredehoeft (Reference 21) was used to simulate groundwater transport around OU3, Hill AFB, Utah. This model has been updated for simulating the transport of non-conservative contaminants. The area of the regional model comprises all the potential sources in OU3 and a substantial area downgradient: with uniformly spaced cells at 250-foot intervals (38 columns and 39 rows). All recharges, discharge, and leakage were determined for each cell based on flow conditions established by the regional groundwater flow model MODFLOW. Values used for permeability and aquifer thickness and other hydrogeologic properties were the same as those for the regional groundwater flow model.

Figure 7 depicts an isoconcentration map of simulated TCE concentration, with contour intervals from 1 μg/l to 21 μg/l, for a retardation factor of 1. Figure 8 is a three-dimensional view of the simulated TCE concentration contours.

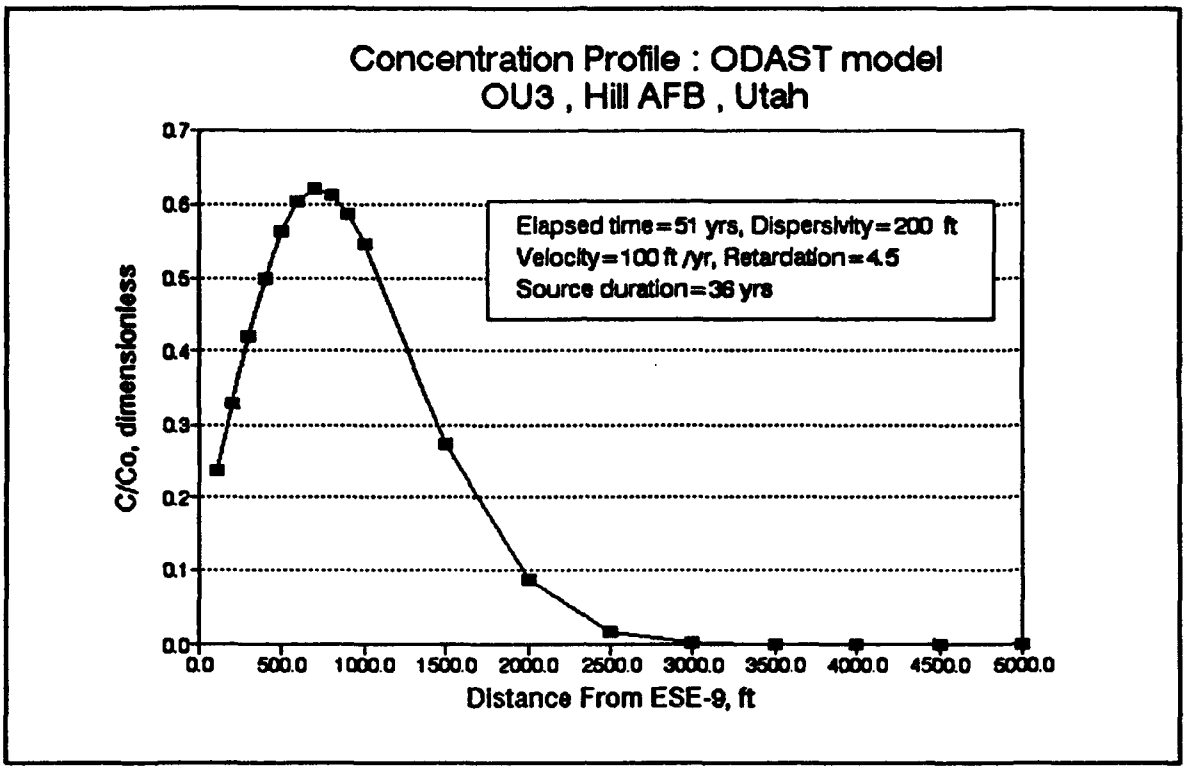

Figure 6. Concentration Profile as Predicted by ODAST

Optimization

This example considers only pump and treat activities as a possible remediation strategy. In addition, the hydraulic conductivity, retardation by sorption and porosity are modeled as random variables. Figure 9 presents a map of the simulated contours of TCE contamination and pumping well placement at Hill AFB. Figure 10 presents the results of evaluating the chance constraint with only 100 iterations and maximum allowable concentrations ranging from 0.1 mg/l to 9.0 mg/l, for 5 different remediation strategies. The results shown here define the cumulative distribution of the contaminant concentration for this situation. For comparison, Figure 10 also presents the cumulative distribution when no remediation activities are implemented at the site.

For any maximum allowable contaminant concentration (*MCL*) a tradeoff relationship can be developed between the cost of remediation and the probability that the remediation strategy will not succeed in containing contaminant concentrations below 5 mg/l. Figure 11 presents this tradeoff relationship. Relationships similar to those presented in Figures 10 and 11 can be used by the Air Force Technical Project Managers as an aid in evaluating and ultimately deciding on a long-term remediation strategy for implementation.

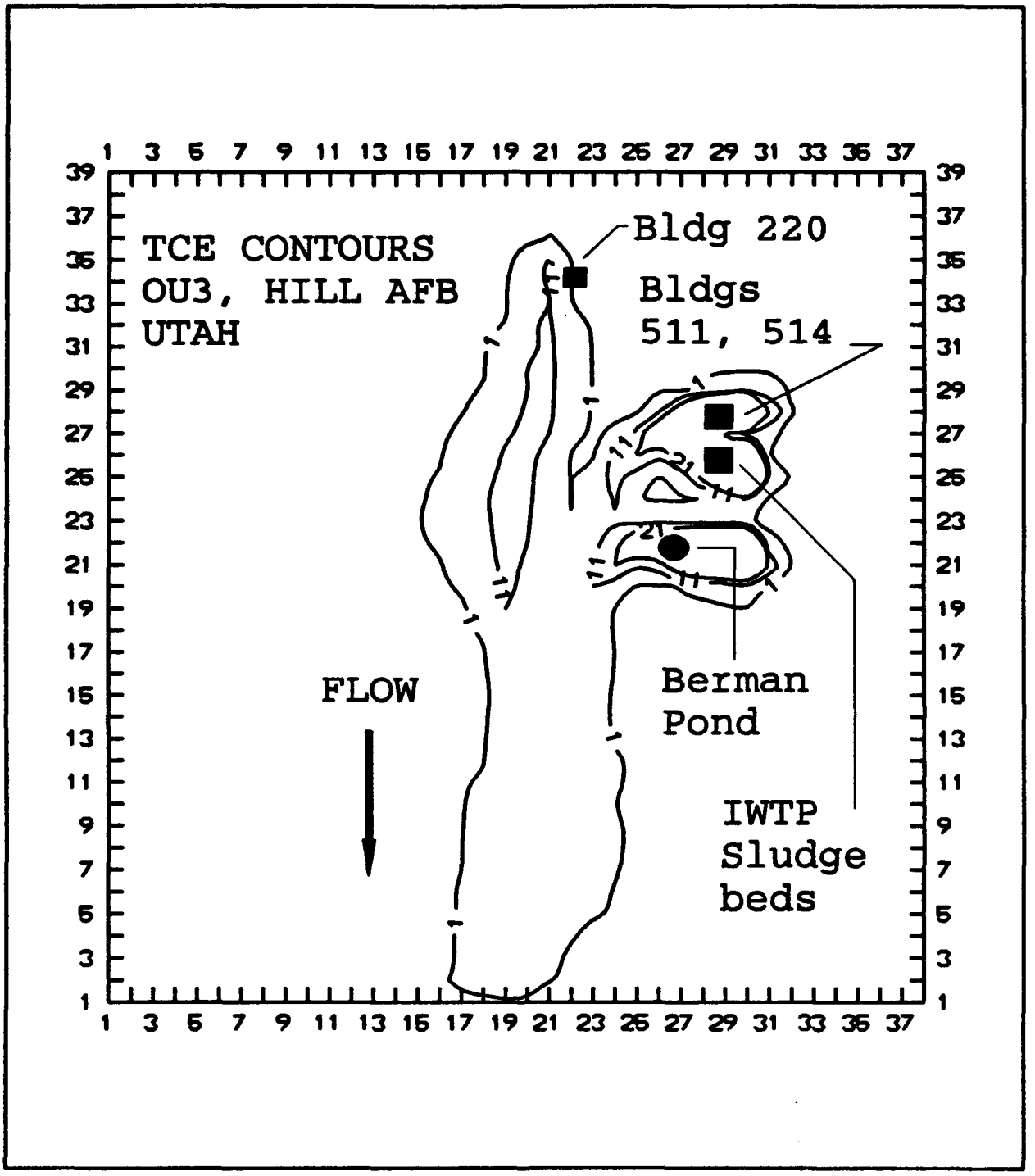

Figure 7. TCE Contours for Operable Unit 3, Hill AFB

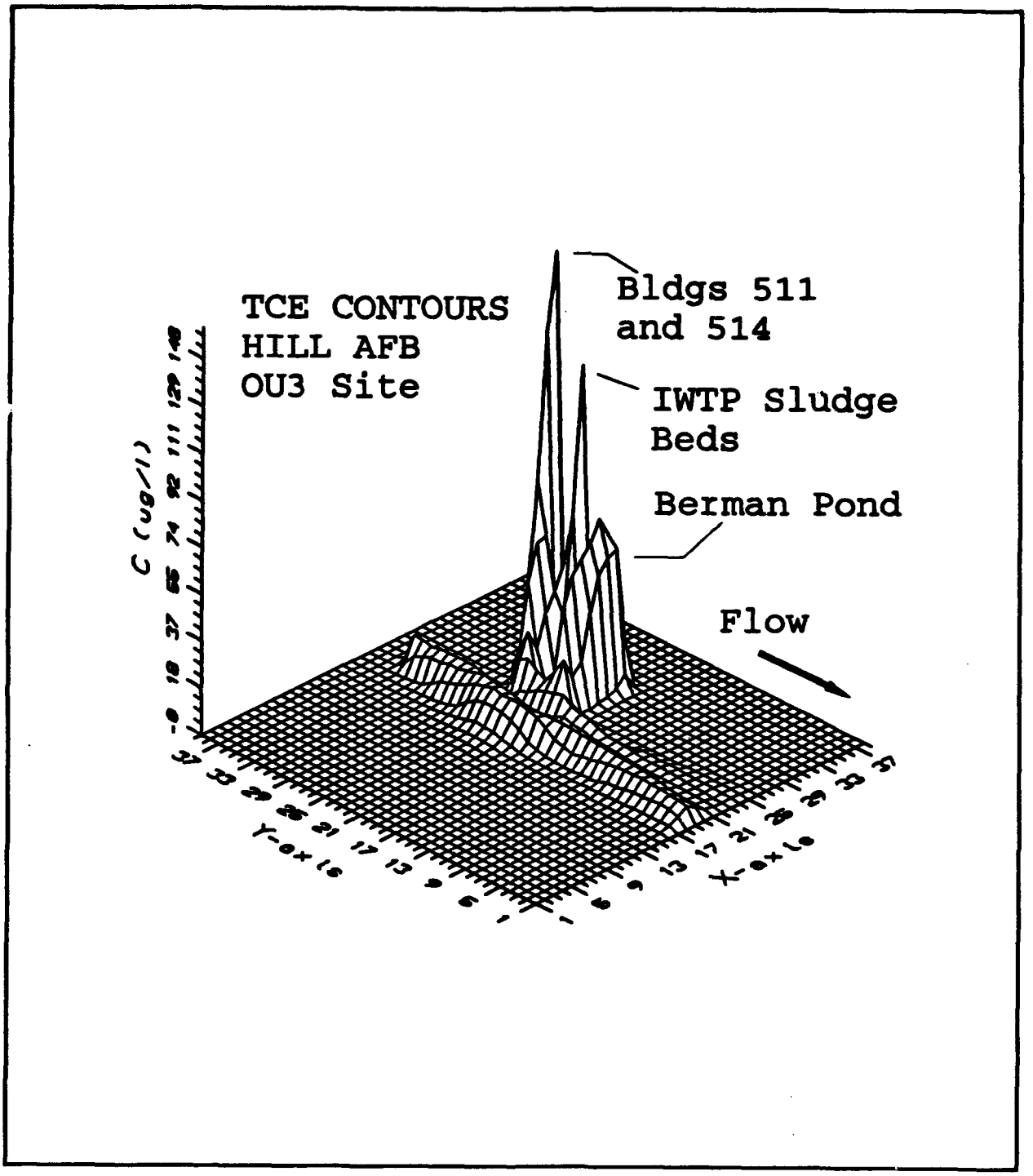

Figure 8. TCE Concentration Surface, Operable Unit 3, Hill AFB, Utah

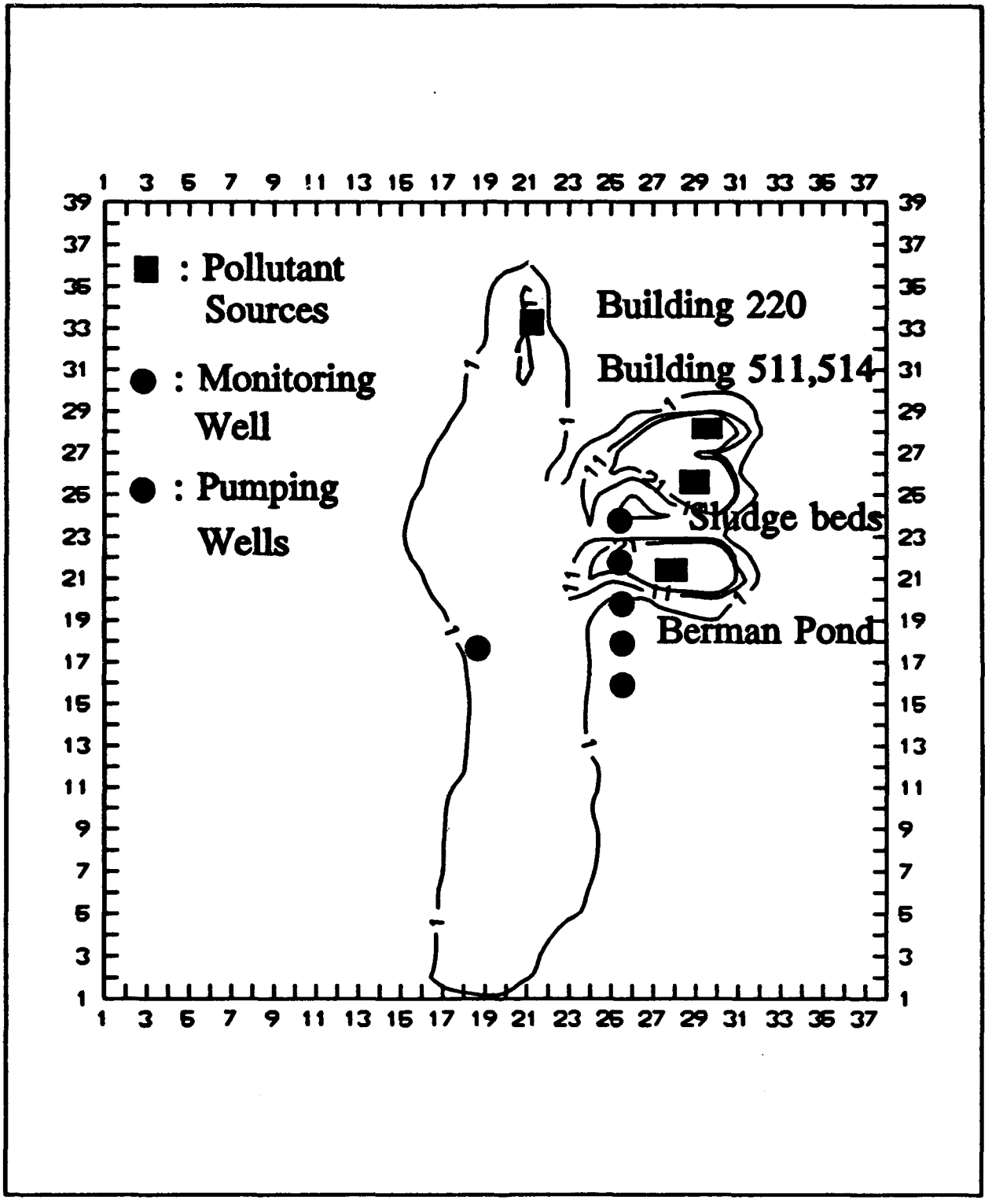

Figure 9. Remediation Well Placement, OU3, Hill AFB

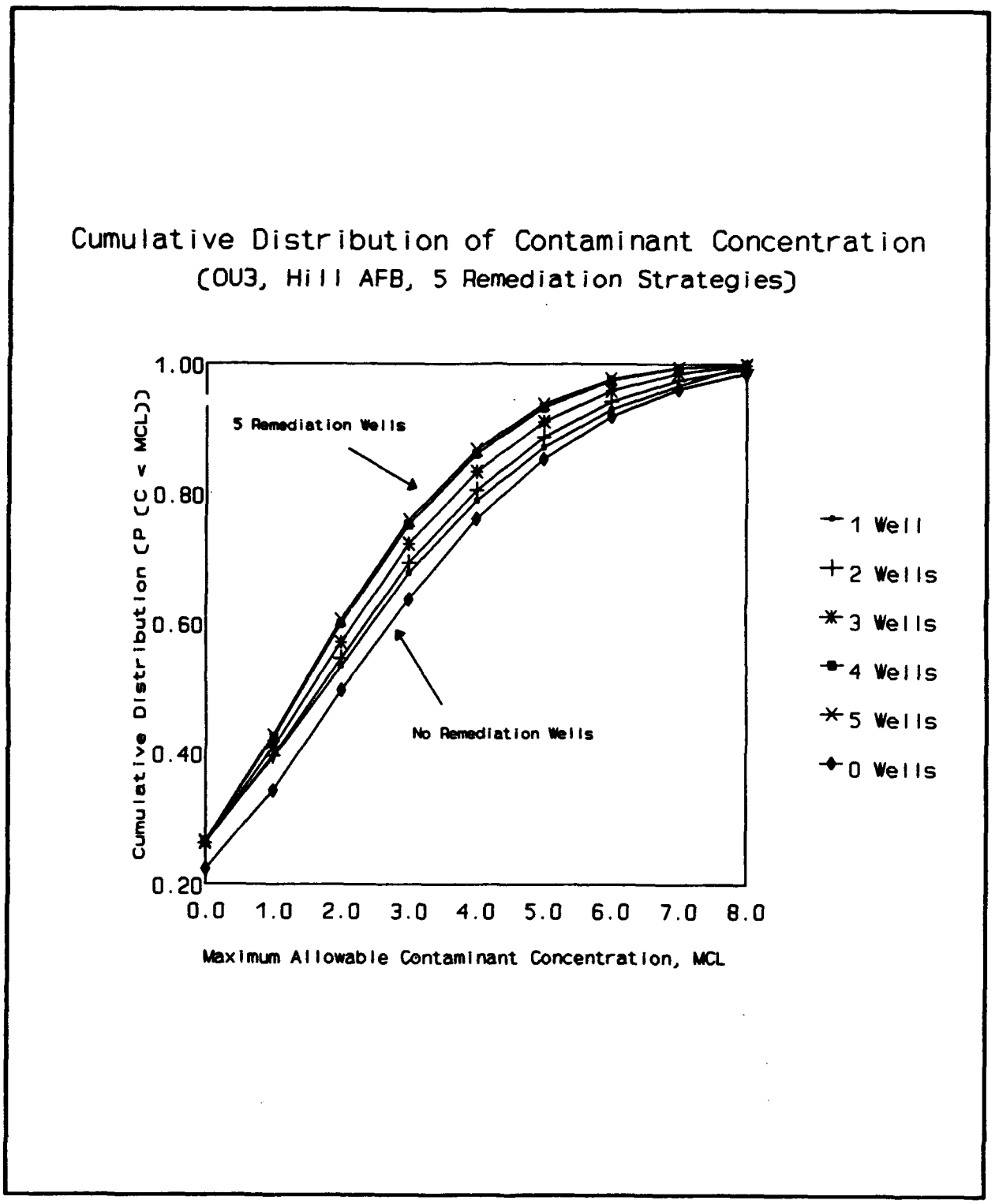

Figure 10. Cumulative Distributions of Contaminant Concentration For Remediation Schemes

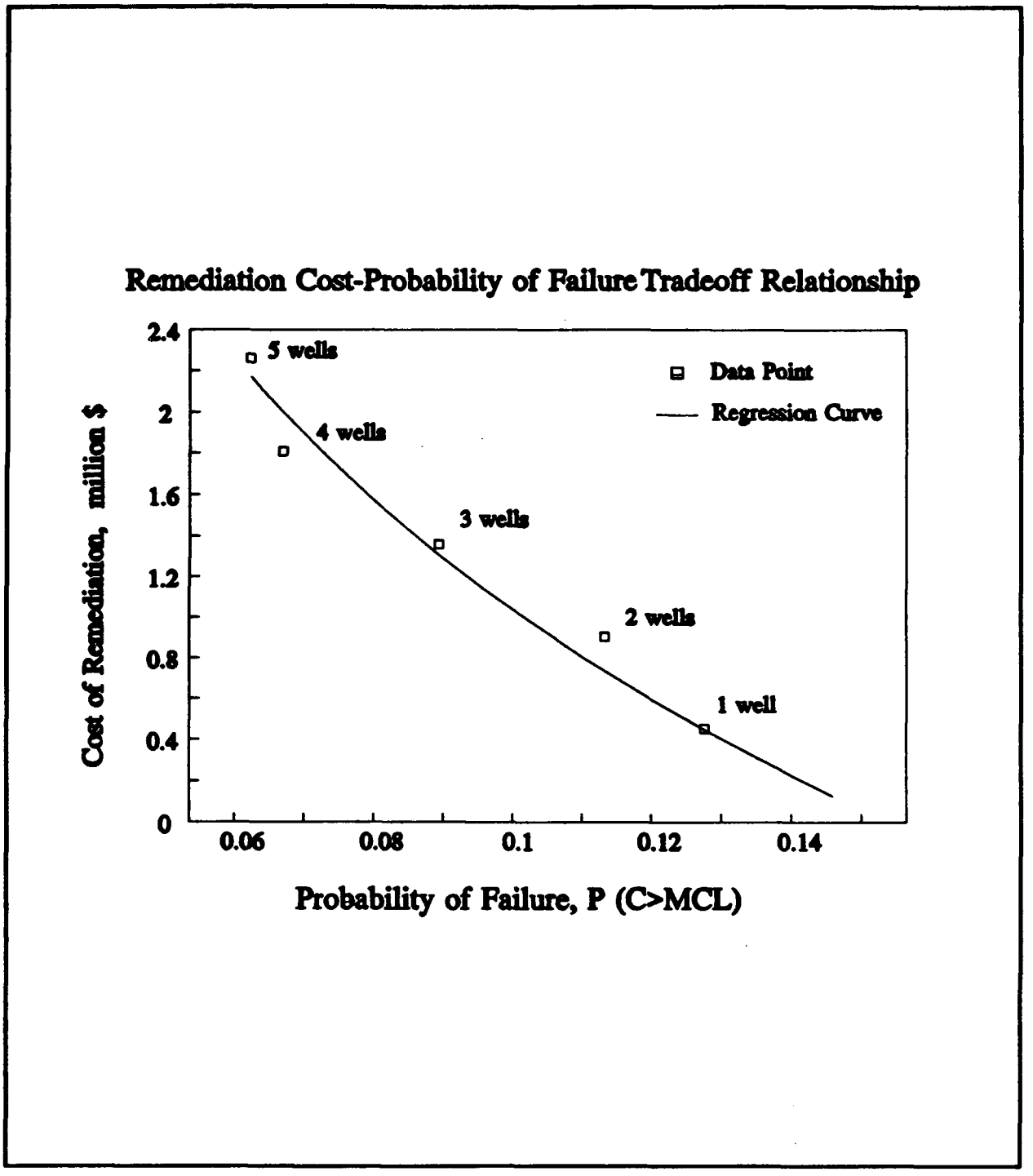

Figure 11. Remediation Cost/Probability of Failure Tradeoff

C. APPLICATION OF RESSQ

RESSQ was used to simulate 2-dimensional advective transport under the injection, extraction, and natural-gradient conditions of the tracer experiments. The field site is in the Moffett Naval Air Station, Mountain View, California (Reference 57). The RESSQ model was used to estimate: (1) the areal extent of the injection fluid front that develops around the injection well and observation wells, (2) the fluid residence times from the injection well to the observation wells, and (3) the degree of recovery of the injected fluid at the extraction well. A sketch of the the well fields is presented in Figure 12, for fluid injection at a rate of 0.5 liter/min at three wells,

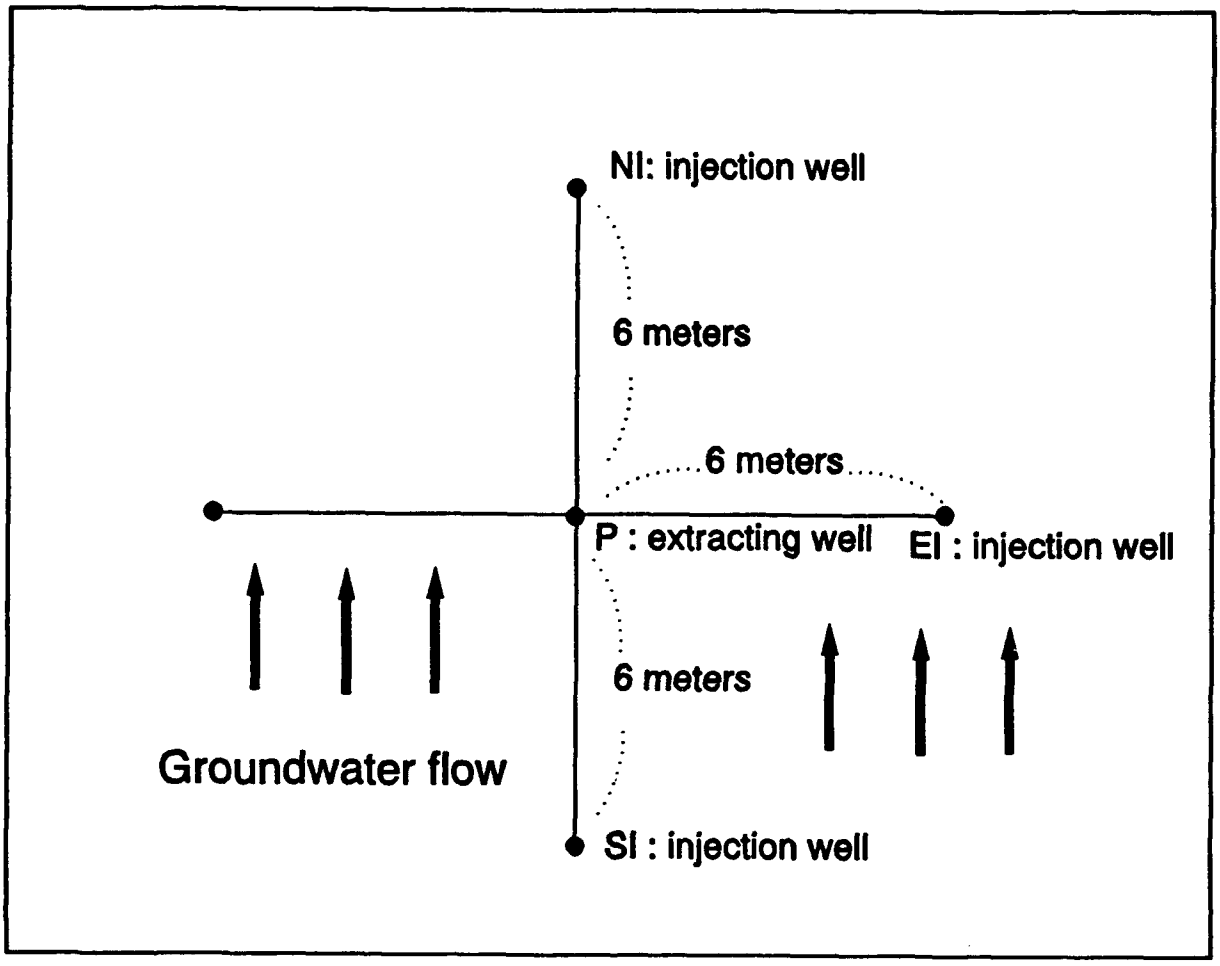

Figure 12. Map of Well Fields at Moffett Site

extraction rate of 8 liters/min, regional ground-water flow of 300 m/yr, a porosity of 0.35, and an aquifer thickness of 1.2 meters.

The results indicate that it is advantageous to use the southern leg for the biorestoration experiments. The reasons are the following: (1) the injected fluid supplying the nutrients becomes less dispersed, and hence a more dense microbial population can be stimulated; (2) by injecting upgradient, the injected tracers and chlorinated hydrocarbons can be most effectively recovered at the extraction well. Figure 13 illustrates the streamlines produced by a graphics post-processor developed specifically for the RESSQ model.

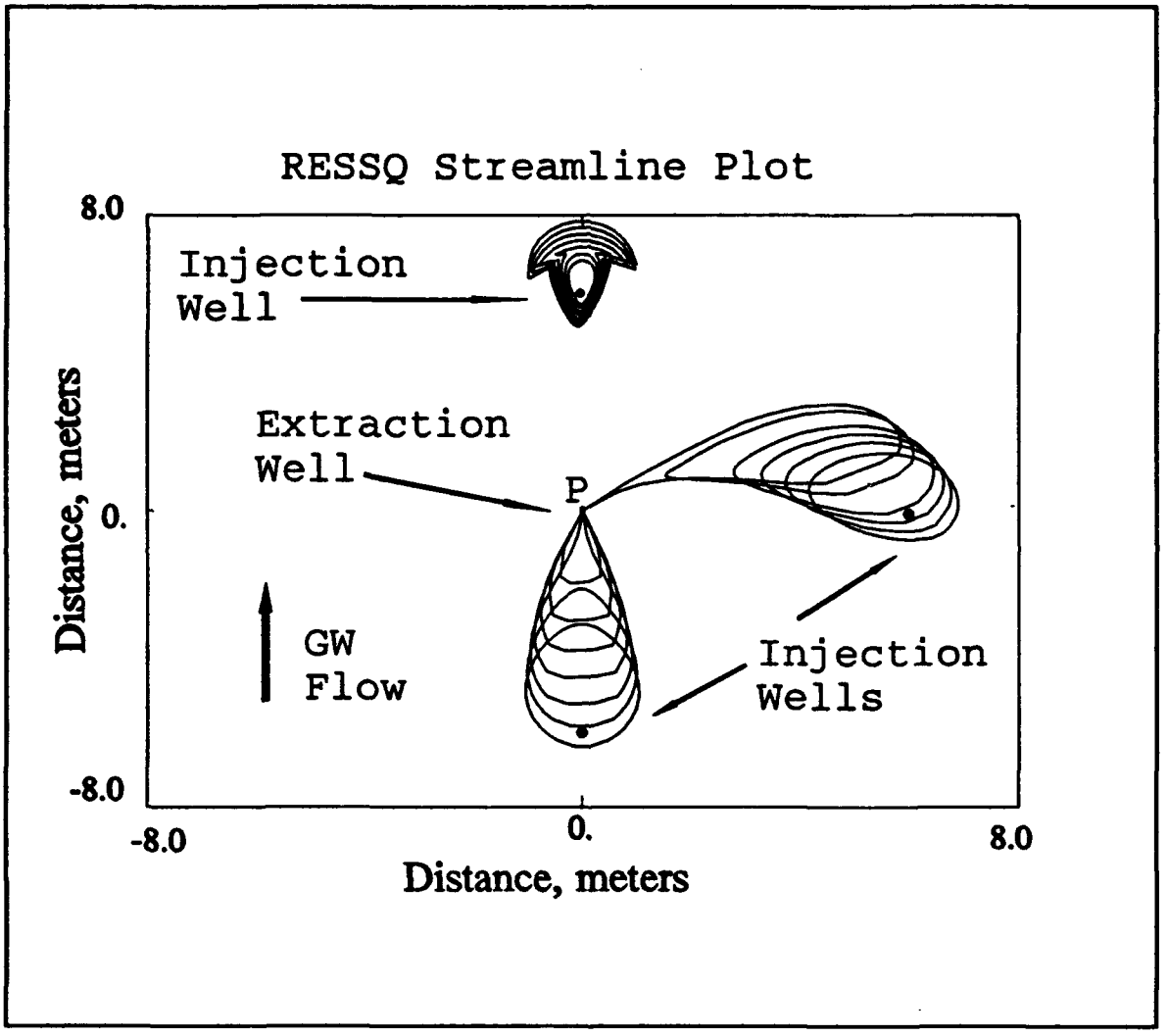

Figure 13. RESSQ Streamline Plot

SECTION IV

CONCLUSIONS

The objective of this research is to develop a groundwater quality and remediation modeling advisory system for use in investigating possible strategies for the cleanup of contamination from hazardous substances, pollutants and contaminants at Air Force sites. In addition, the use of optimization methods is explored for determining optimal remediation for implementation at a specific site. The modeling system was tested successfully for Operable Unit 3, Hill AFB, Utah. The uncertainty associated with groundwater flow and mass transport models was accounted for, not only in the plume prediction itself, but also explicitly in the optimization scheme. The Advisory System also provides guidance to the less experienced users in proper model selection. This report constitutes a technical summary of the methodology and several of the component models. Additional models and refinements to the existing codes are planned for the second phase of the research project, as well as the preparation of a users manual.

Mathematical models are abstractions of the real physical system and/or biochemical processes. Over the past several decades many different models for contaminant transport in porous media, under varying conditions and assumptions, have been proposed and tested. These range from very simple models to very complex models. All of these models, regardless of the complexity of the solution method, require certain assumptions regarding the nature of the transport processes, and therefore can provide only an approximation of the actual spread of contaminants from a given site and the associated risks from human exposure to contaminated groundwater. This situation presents a familiar, yet difficult problem to the analyst and the decision-makers. Sufficient data on the hydrogeology are rarely, if ever, available to apply the most complex codes. The analyst must, whether explicitly or implicitly, choose a transport model based on a trade-off between the presumed greater accuracy of complex models and the less onerous data requirements and easier application of simpler models: an important justification for the development of assistance tools in modeling, despite the concerns that any of these models could still be incorrectly applied by some users. It is ultimately the responsibility of the analyst to assess the results.

Several meetings with Air Force Center for Environmental Excellence (AFCEE) and Air Force Engineering and Services Center (AFESC) staff and representatives of the Installation Restoration Program from other major commands were held to solicit comment from potential users. Their valuable suggestions are being incorporated to make the system more useful and responsive to Air Force needs. There is considerable debate among the modeling community worldwide regarding validation of groundwater models, since they embody scientific hypotheses still under

investigation. The models assembled in this Advisory System within a decision-making framework are still very useful in developing a conceptual model of behavior of contaminants, testing which remedial strategies are the most reasonable, improving data collection in the field by identifying gaps in the database and identifying the most sensitive parameters — even if the user is unable to fully validate, or only partially calibrate the results to field data.

In addition to aiding in the choosing of an appropriate mathematical model for a specific site, the Advisory System is currently being modified to determine efficient or optimal remediation strategies. The optimization routine evaluates tradeoffs between the long-term cost of remediation and the probability the remediation strategy will fail. The development of an efficient, effective and reliable remediation strategy requires a clear understanding of the site characteristics and the remediation actions implemented. In addition, the optimal remediation strategy must consider trade-offs between the remediation cost and the reliability of the remediation strategy. By investigating these trade-offs, the decision maker can more accurately assess remediation needs, feasible remediation strategies and remediation strategy effectiveness. Thus, the complete system incorporates deterministic, stochastic and optimization models within a user-friendly framework.

Long-term remediation costs depend on specific remediation considerations and actions. Examples of possible remediation strategies include pulse pumping and treatment, and continuous pumping and treatment. Potential cost savings are realized by varying the long-term remediation action. The reliability of the long-term remediation strategy represents the likelihood that contaminant concentrations within the groundwater exceeds specified maximums and are modeled as constraints. These two conflicting goals or objectives are weighed against one another using a chance constrained optimization model in which the physical constraints are originally expressed as probabilistic statements.

Using this methodology, optimal groundwater remediation strategies are determined by minimizing the long-term and short-term costs associated with the site remediation. In addition, the optimal remediation strategies are conditioned on the probability that the contaminant concentration at any time does not exceed pre-specified maxima. The actual concentrations at any specified coordinates are calculated by solving the governing differential equations for groundwater contaminant flow in which key site characteristics are expressed as random variables. The resulting optimization model is solved using a second moment formulation combined with Monte Carlo simulation. An example of how the optimization of the remediation process works has been demonstrated for Operable Unit 3, Hill AFB, Utah for five different remedial pumping schemes.

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